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FILE 'REGISTRY' ENTERED AT 11:43:15 ON 06 OCT 2006

=> d his

     FILE 'HCAPLUS' ENTERED AT 10:14:17 ON 06 OCT 2006
L1             1 S US20060116533/PN
                 SEL RN

     FILE 'REGISTRY' ENTERED AT 10:14:42 ON 06 OCT 2006
L2            11 S E1-E11

     FILE 'CASREACT' ENTERED AT 10:15:47 ON 06 OCT 2006
L3             1 S 141:90877/AN
L4               STR
L5            50 S L4
L6               STR L4
L7            24 S L6
L8               SCR 1840
L9            50 S L6 NOT L8
L10              SCR 1839
L11           50 S L6 NOT L10
L12              STR L6
L13           23 S L12
L14              STR
L15              STR
L16              STR
L17              STR
L18              STR
L19           16 S L12 NOT (L14 OR L15 OR L16 OR L17 OR L18)

     FILE 'REGISTRY' ENTERED AT 10:53:39 ON 06 OCT 2006
L20              STR
L21           11 S L20
L22              SCR 1840
L23           35 S L20 NOT L22
L24              SCR 1993 OR 2021 OR 2026 OR 2016
L25              SCR 2043
L26           41 S L20 NOT (L22 OR L24 OR L25)
L27              STR L20
L28              SCR 1918
L29           50 S L27 NOT (L22 OR L24 OR L25 OR L28)
L30              STR
L31              STR L27
L32           50 S L27 NOT L30 NOT (L22 OR L24 OR L25 OR L28)
L33           50 S (L27 NOT L30) NOT (L22 OR L24 OR L25 OR L28)
L34            1 S 7688-25-7/RN
L35            1 S 12150-46-8/RN
L36            1 S 51364-51-3/RN
L37            1 S 87-60-5/RN
L38            1 S 372-39-4/RN
L39            1 S 626-43-7/RN
L40            1 S 108-70-3/RN
L41            1 S 118-69-4/RN
L42            1 S 1013-88-3/RN
L43            1 S 1435-43-4/RN
L44            1 S 865-48-5/RN
L45           50 S (L27 NOT L30) NOT (L24 OR L25 OR L28)
L46              STR
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L48          38 S (L27 NOT (L46 OR L30)) NOT (L24 OR L25 OR L28)
L49       13084 S (L27 NOT (L46 OR L30)) NOT (L24 OR L25 OR L28) FUL
L50           3 S L49 AND L2
                SAV L49 VAL801/A

     FILE 'HCAPLUS' ENTERED AT 11:36:53 ON 06 OCT 2006
L51       40051 S L49
L52        1529 S L37-L39
L53        2116 S L40 OR L41 OR L43
L54         789 S L42
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L56          76 S L52 AND L53
L57          17 S L56 AND PREP/RL
L58       38522 S L51 NOT L52
L59           0 S L58 AND L53 AND L54
L60         175 S L58 AND L53
L61          39 S L60 AND PREP/RL
L62          56 S L57 OR L61
L63           1 S L62 AND L1
L64          55 S L62 AND (1840-2002)/PRY,AY,PY


=> d que
L24             SCR 1993 OR 2021 OR 2026 OR 2016
L25             SCR 2043
L27             STR
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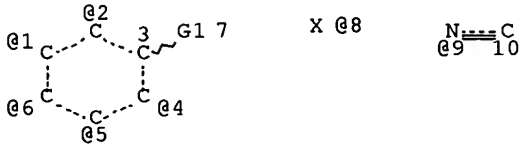


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VAR G1=NH2/NH3/9
VPA 8-2/1/6/5/4 U
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DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS  10

STEREO ATTRIBUTES: NONE
L28             SCR 1918
L30             STR
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NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED
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GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 2

STEREO ATTRIBUTES: NONE
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L38 1 SEA FILE=REGISTRY ABB=ON 372-39-4/RN
L39 1 SEA FILE=REGISTRY ABB=ON 626-43-7/RN
L40 1 SEA FILE=REGISTRY ABB=ON 108-70-3/RN
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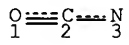
L46 STR



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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
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NUMBER OF NODES IS 3

STEREO ATTRIBUTES: NONE
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L53 2116 SEA FILE=HCAPLUS ABB=ON L40 OR L41 OR L43
L56 76 SEA FILE=HCAPLUS ABB=ON L52 AND L53
L57 17 SEA FILE=HCAPLUS ABB=ON L56 AND PREP/RL
L58 38522 SEA FILE=HCAPLUS ABB=ON L51 NOT L52
L60 175 SEA FILE=HCAPLUS ABB=ON L58 AND L53
L61 39 SEA FILE=HCAPLUS ABB=ON L60 AND PREP/RL
L62 56 SEA FILE=HCAPLUS ABB=ON L57 OR L61
L64 55 SEA FILE=HCAPLUS ABB=ON L62 AND (1840-2002)/PRY,AY,PY

=> fil hcap
FILE 'HCAPLUS' ENTERED AT 11:43:26 ON 06 OCT 2006

=>d l64 1-55 ibib abs hitstr hitind

L64 ANSWER 1 OF 55 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:534164 HCAPLUS Full-text
DOCUMENT NUMBER: 141:90877
TITLE: Process for preparation of substituted halogenated anilines
INVENTOR(S): Smith, Jonathan O.; Petruska, Melissa A.; Longlet, Jon J.
PATENT ASSIGNEE(S): BASF Aktiengesellschaft, Germany
SOURCE: PCT Int. Appl., 11 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004054961	A1	20040701	WO 2003-EP14354	2003 1216
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W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003298961	A1	20040709	AU 2003-298961	2003 1216
			<--	
EP 1575898	A1	20050921	EP 2003-813132	2003 1216
			<--	
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003017311	A	20051108	BR 2003-17311	2003 1216
			<--	
CN 1723189	A	20060118	CN 2003-80105713	2003 1216
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JP 2006509821	T2	20060323	JP 2004-560446	2003 1216
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US 2006116533	A1	20060601	US 2005-537801	2005 0607
			<--	
PRIORITY APPLN. INFO.:			US 2002-433847P P	2002 1216
			<--	
			WO 2003-EP14354 W	2003 1216

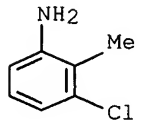
OTHER SOURCE(S): CASREACT 141:90877; MARPAT 141:90877

AB A process for preparation of substituted halogenated anilines from substituted halogenated 1-chlorobenzenes comprises (a) reacting a substituted halogenated 1-chlorobenzene selectively with an imine in the presence of a transition

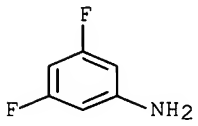
metal catalyst complex and a base to form an N-aryl imine; (b) hydrolyzing the N-aryl imine; and (c) isolating the substituted halogenated aniline. Thus, heating 2,6-dichlorotoluene, benzophenone imine, tris(dibenzylideneacetone)dipalladium(0), 1,1'-bis(diphenylphosphino)ferrocene, and Na tert-butoxide in xylene, and hydrolyzing the resulting reaction product gave 3-chloro-2-methylaniline in 75.5% yield.

IT **87-60-5P**, 3-Chloro-2-methylaniline **372-39-4P**, 3,5-Difluoroaniline **626-43-7P**, 3,5-Dichloroaniline
(preparation of substituted halogenated anilines from substituted chlorobenzenes)

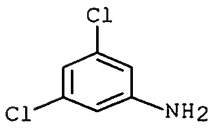
RN 87-60-5 HCAPLUS
CN Benzenamine, 3-chloro-2-methyl- (9CI) (CA INDEX NAME)



RN 372-39-4 HCAPLUS
CN Benzenamine, 3,5-difluoro- (9CI) (CA INDEX NAME)

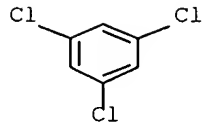


RN 626-43-7 HCAPLUS
CN Benzenamine, 3,5-dichloro- (9CI) (CA INDEX NAME)

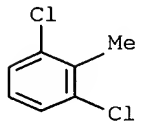


IT **108-70-3**, 1,3,5-Trichlorobenzene **118-69-4**, 2,6-Dichlorotoluene **1435-43-4**, 1-Chloro-3,5-difluorobenzene
(preparation of substituted halogenated anilines from substituted chlorobenzenes)

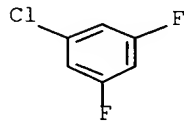
RN 108-70-3 HCAPLUS
CN Benzene, 1,3,5-trichloro- (8CI, 9CI) (CA INDEX NAME)



RN 118-69-4 HCAPLUS
CN Benzene, 1,3-dichloro-2-methyl- (9CI) (CA INDEX NAME)



RN 1435-43-4 HCAPLUS
CN Benzene, 1-chloro-3,5-difluoro- (7CI, 8CI, 9CI) (CA INDEX NAME)



IC ICM C07C209-52
ICS C07C211-45; B01J023-44
CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)
Section cross-reference(s): 25
IT **87-60-5P**, 3-Chloro-2-methylaniline **372-39-4P**,
3,5-Difluoroaniline **626-43-7P**, 3,5-Dichloroaniline
(preparation of substituted halogenated anilines from substituted chlorobenzenes)
IT **108-70-3**, 1,3,5-Trichlorobenzene **118-69-4**,
2,6-Dichlorotoluene 1013-88-3, Benzophenone imine
1435-43-4, 1-Chloro-3,5-difluorobenzene
(preparation of substituted halogenated anilines from substituted chlorobenzenes)
REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L64 ANSWER 2 OF 55 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:971587 HCAPLUS Full-text
DOCUMENT NUMBER: 140:4846
TITLE: Process for preparation of 1,3,5-triaminobenzene and its hydrolysis to high purity phloroglucinol
INVENTOR(S): Ismaili, Lhassane; Refouvelet, Bernard; Xicluna, Alain
PATENT ASSIGNEE(S): Seranalis, Fr.
SOURCE: Fr. Demande, 21 pp.

CODEN: FRXXBL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2840608	A1	20031212	FR 2002-7177	20020611
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FR 2840608	B1	20050701		
CA 2487973	AA	20031218	CA 2003-2487973	20030606
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WO 2003104194	A1	20031218	WO 2003-FR1703	20030606
			<--	

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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

AU 2003260577	A1	20031222	AU 2003-260577	20030606
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EP 1511726	A1	20050309	EP 2003-757119	20030606
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EP 1511726	B1	20051109		

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BR 2003011786	A	20050329	BR 2003-11786	20030606
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US 2005165256	A1	20050728	US 2003-517716	20030606
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CN 1668586	A	20050914	CN 2003-816631	20030606
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AT 309214	E	20051115	AT 2003-757119	2003

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JP 2005534659	T2	20051117	JP 2004-511264	
				2003
				0606
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ES 2252690	T3	20060516	ES 2003-3757119	
				2003
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PRIORITY APPLN. INFO.:			FR 2002-7177	A
				2002
				0611
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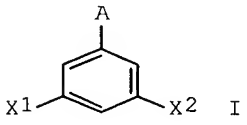
			WO 2003-FR1703	W
				2003
				0606

OTHER SOURCE(S): CASREACT 140:4846; MARPAT 140:4846
GI

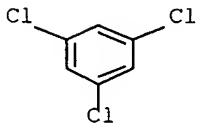


I

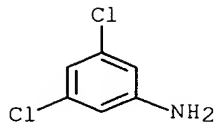
AB 1,3,5-Triaminobenzene is prepared by treatment of I (A = halo, NH2; X1, X2 = halo) with NH3 in the presence of a copper salt or oxide catalyst at 150-250° and >35 bar; subsequent hydrolysis by HCl gives phloroglucinol. Thus, reaction of 1,3,5- trichlorobenzene with NH3 in the presence of copper iodide at 180°/40 bar, followed by hydrolysis with HCl at 120°, gave phloroglucinol in 40% yield.

IT **108-70-3**, 1,3,5-Trichlorobenzene **626-43-7**, 3,5-Dichloroaniline
(1,3,5-benzenetriamine and phloroglucinol via copper iodide catalyzed amination of halobenzenes and subsequent hydrolysis)

RN 108-70-3 HCAPLUS
CN Benzene, 1,3,5-trichloro- (8CI, 9CI) (CA INDEX NAME)



RN 626-43-7 HCAPLUS
CN Benzenamine, 3,5-dichloro- (9CI) (CA INDEX NAME)

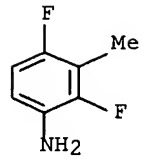


IC ICM C07C211-49
ICS C07C039-10; A61K031-05; A61P021-00; A61P025-08
CC 25-10 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
IT **108-70-3**, 1,3,5-Trichlorobenzene **626-43-7**, 3,5-Dichloroaniline
(1,3,5-benzenetriamine and phloroglucinol via copper iodide catalyzed amination of halobenzenes and subsequent hydrolysis)
REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

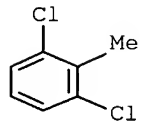
L64 ANSWER 3 OF 55 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:929516 HCAPLUS Full-text
DOCUMENT NUMBER: 139:381248
TITLE: Preparation of 2,4,5-trifluoro-3-methyl-6-nitrobenzoic acid
INVENTOR(S): Hayashi, Kazuhiko
PATENT ASSIGNEE(S): Asahi Glass Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 10 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2003335730	A2	20031128	JP 2002-138590 <--	20020514
PRIORITY APPLN. INFO.:			JP 2002-138590 <--	20020514

OTHER SOURCE(S): MARPAT 139:381248
AB Title compound (I), useful as an intermediate for quinolone bactericides, is prepared from 2,6-dichlorotoluene (II). 2,3,6-Trifluorotoluene (prepared from II in 4 steps) was acylated by AcCl in the presence of AlCl3 at 105° for 1 h to give 83% 2,3,6-trifluoro-5-acetyltoluene, which was nitrated by KNO3/H2SO4 and treated with aqueous NaClO under reflux for 2 h to give I.
IT **76350-70-4P**
(preparation of trifluoromethylnitrobenzoic acid from dichlorotoluene as intermediate for quinolone bactericides)
RN 76350-70-4 HCAPLUS
CN Benzenamine, 2,4-difluoro-3-methyl- (9CI) (CA INDEX NAME)



IT **118-69-4**, 2,6-Dichlorotoluene
(preparation of trifluoromethylnitrobenzoic acid from dichlorotoluene as intermediate for quinolone bactericides)
RN 118-69-4 HCAPLUS
CN Benzene, 1,3-dichloro-2-methyl- (9CI) (CA INDEX NAME)



IC ICM C07C201-12
ICS C07C201-08; C07C205-58
CC 25-17 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 1
IT 29682-46-0P, 2,6-Dichloro-3-nitrotoluene **76350-70-4P**
79562-49-5P, 2,6-Difluoro-3-nitrotoluene 83277-23-0P,
2,4-Dichloro-3-methylbenzoic acid 99938-06-4P,
2,6-Dichloro-3-trichloromethyltoluene 103877-66-3P
119916-24-4P 119916-25-5P, 2,3,6-Trifluorotoluene 174637-91-3P
181216-49-9P 625124-34-7P 625124-35-8P 625124-36-9P
625124-37-0P 625124-38-1P 625124-40-5P
(preparation of trifluoromethylnitrobenzoic acid from dichlorotoluene as intermediate for quinolone bactericides)
IT **118-69-4**, 2,6-Dichlorotoluene
(preparation of trifluoromethylnitrobenzoic acid from dichlorotoluene as intermediate for quinolone bactericides)

L64 ANSWER 4 OF 55 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:696882 HCAPLUS Full-text
DOCUMENT NUMBER: 139:230615
TITLE: Preparation of benzofurans and benzothiophenes useful in the treatment of hyperproliferative disorders
INVENTOR(S): Zhang, Chengzhi; Burke, Michael; Chen, Zhi; Dumas, Jacques; Fan, Dongping; Fan, Jianmei; Hatoum-Mokdad, Holia; Jones, Benjamin D.; Ladouceur, Gaetan; Lee, Wendy; Phillips, Barton
PATENT ASSIGNEE(S): Bayer Pharmaceuticals Corporation, USA
SOURCE: PCT Int. Appl., 138 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003072561	A1	20030904	WO 2003-US5396	2003 0221
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
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EP 1487813	A1	20041222	EP 2003-709265	2003 0221
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CN 1639145	A	20050713	CN 2003-804442	2003 0221
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JP 2006507215	T2	20060302	JP 2003-571267	2003 0221
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BR 2003007905	A	20060404	BR 2003-7905	2003 0221
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ZA 2004007482	A	20050919	ZA 2004-7482	2004 0917
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NO 2004003952	A	20041022	NO 2004-3952	2004 0921

PRIORITY APPLN. INFO.:	<-- US 2002-359011P	P	2002 0222
	<-- US 2002-399886P	P	2002 0731
	<-- WO 2003-US5396	W	2003 0221

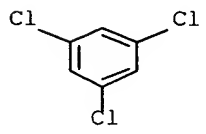
OTHER SOURCE(S): MARPAT 139:230615
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

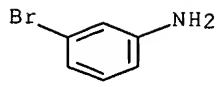
AB Title compds. I [wherein X = O, S; R1 = H, alkyl, (CO)alkyl, benzoyl; R2 = (un)substituted Ph, naphthyl, (un)substituted heterocyclyl; R3 = H, OH, CN, alkyl, alkoxy, halo, haloalkyl, haloalkoxy; R4 = piperonyl, (un)substituted heterocyclyl, Ph and naphthyl; R5, R6 = independently H, OH, CN, alkyl, alkoxy, halo, haloalkyl and haloalkoxy; and their pharmaceutically acceptable salts or esters] were prepared as antitumor agents for treatment of hyperproliferative disorders. For example, II was prepared from 2-bromo-3'-methoxy-acetophenone by cyclocondensation with acetamide at 110° for 40 h, demethylation in DCM at room temperature for 2 h, reaction with paraformaldehyde in CH3CN/TEA in the presence of MgCl2 at reflux for 17 h, reaction with nitroethane in AcOH/AcONa at reflux for 17 h, and K2CO3-catalyzed cyclocondensation of the resultant nitrile with 2-methoxyphenacyl bromide in anhydrous DMF. III was prepared, in 28.2% yield, by Pd-cross coupling of (3-amino-6-iodo-1-benzothiophene-2-yl)(2,4-dichlorophenyl)methanone with pyridine-3-boronic acid in 1,2-dimethoxyethane at 80° for 18 h. I showed a significant inhibition of tumor cell proliferation in the adherent tumor cell proliferation assay (no data). Thus, I and their formulations are useful as antitumor agents (no data).

IT **108-70-3**, 1,3,5-Trichlorobenzene **591-19-5**, 3-Bromoaniline **626-01-7**, 3-Iodoaniline
(preparation of benzofurans and benzothiophenes for treatment of hyper-proliferative disorders)

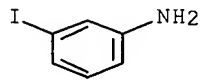
RN 108-70-3 HCAPLUS
CN Benzene, 1,3,5-trichloro- (8CI, 9CI) (CA INDEX NAME)



RN 591-19-5 HCAPLUS
CN Benzenamine, 3-bromo- (9CI) (CA INDEX NAME)



RN 626-01-7 HCAPLUS
CN Benzenamine, 3-iodo- (9CI) (CA INDEX NAME)

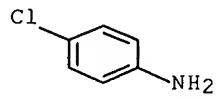


IC ICM C07D307-82
ICS C07D333-66; C07D413-04; C07D417-04; C07D405-04; C07D409-04; C07D409-14; C07D405-14; C07D405-10; A61K031-343; A61P035-00
CC 27-9 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1, 63
IT **108-70-3**, 1,3,5-Trichlorobenzene 109-85-3, 2-Methoxyethylamine 110-91-8, Morpholine, reactions 121-71-1, 1-(3-Hydroxyphenyl)ethanone 288-32-4, Imidazole, reactions 350-03-8, 3-Acetylpyridine 372-48-5, 2-Fluoropyridine 497-25-6, 2-Oxazolidone 580-51-8, 3-Phenylphenol **591-19-5**, 3-Bromoaniline 591-20-8, 3-Bromophenol 625-45-6, Methoxyacetic acid **626-01-7**, 3-Iodoaniline 626-02-8, 3-Iodophenol 696-40-2, 3-Iodobenzylamine 823-78-9, 1-Bromo-3-bromomethylbenzene 1692-25-7, Pyridine-3-boronic acid 1711-09-7, 3-Bromobenzoyl chloride 2142-63-4, 3-Bromoacetophenone 2476-37-1 2725-82-8, 1-Bromo-3-ethylbenzene 2905-24-0, 3-Bromobenzenesulfonyl chloride 4023-34-1, Cyclopropanecarbonyl chloride 4252-78-2, 2-Chloro-1-(2,4-dichlorophenyl)ethanone 5000-65-7, 2-Bromo-3'-methoxyacetophenone 6320-01-0, 3-Bromobenzenethiol 6972-41-4, 3-Diethylaminopropionic acid 7797-83-3, Benzo[1,3]dioxole-4-carboxaldehyde 16419-60-6, 2-Methylphenylboronic acid 16420-13-6, Dimethylthiocarbamoyl chloride 25015-63-8, Pinacolborane 30318-99-1, 3-Bromo-4-methylthiophene 30418-59-8, 3-Aminophenylboronic acid 31938-07-5, 3-Bromophenylacetonitrile 31949-21-0, 2-Methoxyphenacyl bromide 33733-73-2, 3-Bromothioanisole 38749-79-0, 3-Bromo-2-methylpyridine 57044-25-4, (R)-(+)-Glycidol 61397-54-4, 2-Bromo-1-(2-chloro-4-fluorophenyl)ethanone 61858-38-6, 3-Iodophenacyl bromide 73183-34-3 78887-39-5, 3-Acetamidobenzeneboronic acid 105942-08-3, 4-Bromo-2-fluorobenzonitrile 112279-61-5, 4-Amino-2,5-difluorobenzonitrile 158063-66-2, 4-Trifluoromethylnicotinic acid 454473-64-4, Methyl 2-hydroxy-4-(1H-pyrrol-1-yl)benzenecarboxylate
(preparation of benzofurans and benzothiophenes for treatment of hyper-proliferative disorders)
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

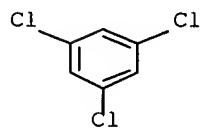
L64 ANSWER 5 OF 55 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:308237 HCAPLUS Full-text
DOCUMENT NUMBER: 137:33373
TITLE: Sequential Photostimulated Reactions of Trimethylstannyl Anions with Aromatic Compounds Followed by Palladium-Catalyzed Cross-Coupling Processes
AUTHOR(S): Corsico, Eduardo F.; Rossi, Roberto A.
CORPORATE SOURCE: INFIQC, Departamento de Quimica Organica, Facultad de Ciencias Quimicas, Universidad Nacional de Cordoba, Cordoba, 5000, Argent.
SOURCE: Journal of Organic Chemistry (**2002**), 67(10), 3311-3316
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:33373

AB The photostimulated reactions of several mono-, di-, and trichloroarenes and aryltrimethylammonium salts with Me3Sn- ions in liquid ammonia gave good yields of stannanes by the SRN1 mechanism. If the chloroarenes are not soluble in liquid ammonia, diglyme is another solvent to perform these reactions. The stannanes thus obtained can be arylated by further reaction with haloarenes through palladium-catalyzed reactions. If the palladium-catalyzed reaction is performed with a chloroiodoarene as substrate, the stannane reacts faster by the C-I bond via chemoselective cross-coupling reaction to give a chloroarene as product, which can be further arylated by a consecutive SRN1-Stille reaction or react with other substrates by another palladium-catalyzed reaction. These sequential reactions can also be performed with substrates with two leaving groups to give products in high yields.

IT **106-47-8**, 4-Chloroaniline, reactions
(photochem. trimethylstannylation of)
RN 106-47-8 HCAPLUS
CN Benzenamine, 4-chloro- (9CI) (CA INDEX NAME)

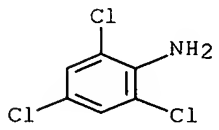


IT **108-70-3**, 1,3,5-Trichlorobenzene
(sequential photostimulated reactions of trimethylstannyl anions with aromatic compds. followed by palladium-catalyzed cross-coupling processes)
RN 108-70-3 HCAPLUS
CN Benzene, 1,3,5-trichloro- (8CI, 9CI) (CA INDEX NAME)

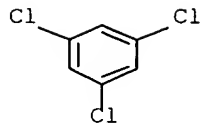


CC 29-8 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 25
IT **106-47-8**, 4-Chloroaniline, reactions
(photochem. trimethylstannylation of)
IT 90-13-1, 1-Chloronaphthalene 98-04-4, Phenyltrimethylammonium iodide **108-70-3**, 1,3,5-Trichlorobenzene 541-73-1, 1,3-Dichlorobenzene 623-03-0, p-Chlorobenzonitrile 1066-45-1, Chlorotrimethylstannane
(sequential photostimulated reactions of trimethylstannyl anions with aromatic compds. followed by palladium-catalyzed cross-coupling processes)
REFERENCE COUNT: 54 THERE ARE 54 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L64 ANSWER 6 OF 55 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:255497 HCAPLUS Full-text
DOCUMENT NUMBER: 137:124949
TITLE: A newly developed synthesis of 1,3,5-trichlorobenzene (sym. TCB) from aniline
AUTHOR(S): Mehilal; Salunke, R. B.; Agrawal, J. P.
CORPORATE SOURCE: High Energy Materials Research Laboratory, Pune, 411 021, India
SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (**2002**), 41B(3), 604-607
CODEN: IJSBDB; ISSN: 0376-4699
PUBLISHER: National Institute of Science Communication
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:124949
AB 1,3,5-Trichlorobenzene (sym. TCB) was synthesized by diazotization of 2,4,6-trichloroaniline (sym. TCA) (by converting aniline into anilinium chloride followed by its chlorination) in the presence of H2SO4/NaNO2 and H3PO2. The reaction parameters for the synthesis of both sym. TCA as well as sym. TCB also were established to get better purity and higher yields. Different reaction parameters for the nitration of sym. TCB to get 1,3,5-trichloro-2,4,6-trinitrobenzene (TCTNB) and its amination to get pure 1,3,5-triamino-2,4,6-trinitrobenzene (TATB) also were established. A comparison of properties of TATB obtained from imported sym. TCB and from laboratory prepared sym. TCB validates the product.
IT **634-93-5P**, 2,4,6-Trichloroaniline
(preparation of 1,3,5-trichlorobenzene from aniline)
RN 634-93-5 HCAPLUS
CN Benzenamine, 2,4,6-trichloro- (9CI) (CA INDEX NAME)

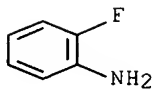


IT **108-70-3P**, 1,3,5-Trichlorobenzene
(preparation of 1,3,5-trichlorobenzene from aniline)
RN 108-70-3 HCAPLUS
CN Benzene, 1,3,5-trichloro- (8CI, 9CI) (CA INDEX NAME)

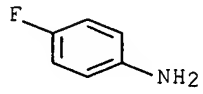


CC 25-3 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 45, 50
IT 142-04-1P, Anilinium chloride **634-93-5P**,
2,4,6-Trichloroaniline
(preparation of 1,3,5-trichlorobenzene from aniline)
IT **108-70-3P**, 1,3,5-Trichlorobenzene
(preparation of 1,3,5-trichlorobenzene from aniline)
REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

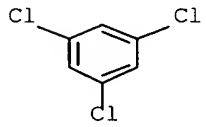
L64 ANSWER 7 OF 55 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:72699 HCAPLUS Full-text
DOCUMENT NUMBER: 134:280671
TITLE: Synthesis of 2,3-dihydroindoles, indoles, and anilines by transition metal-free amination of aryl chlorides
AUTHOR(S): Beller, Matthias; Breindl, Claudia; Riermeier, Thomas H.; Tillack, Annegret
CORPORATE SOURCE: Institut fuer Organische Katalyseforschung, Universitaet Rostock e. V., Rostock, 18055, Germany
SOURCE: Journal of Organic Chemistry (**2001**), 66(4), 1403-1412
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:280671
AB Aliphatic and aromatic amines RNH2 [R = Ph, 2-MeOC6H4, 4-FC6H4, 3-F3CC6H4, 4-PhC6H4, 2-FC6H4, 1-anthracenyl, Bu, Me3C, Ph(CH2)2, EtO(CH2)3] react with 2- and 3-chlorostyrenes in the presence of potassium tert-butoxide to give N-substituted 2,3-dihydroindoles in good yields. The combination of this domino-amination protocol with a suitable dehydrogenation reaction gives access to pharmacol. interesting indoles in a one-pot procedure. Overall product yields of N-substituted indoles >50% are obtained by this method starting from com. available substrates. In addition to the intramol. base-promoted amination of aromatic C-Cl bonds, metal-free intermol. aminations of aryl chlorides, e.g., PhCl, with primary and secondary amines, e.g., piperidine, are described. The use of potassium tert-butoxide as base allows the synthesis of various anilines in good to excellent yields. Due to the formation of aryne intermediates, either N-substituted anilines or meta-substituted anilines are produced with excellent selectivities.
IT **348-54-9**, 2-Fluoroaniline **371-40-4**,
4-Fluoroaniline
(preparation of 2,3-dihydroindoles and indoles by palladium-free amination-cyclization or amination of chlorostyrenes)
RN 348-54-9 HCAPLUS
CN Benzenamine, 2-fluoro- (9CI) (CA INDEX NAME)



RN 371-40-4 HCAPLUS
CN Benzenamine, 4-fluoro- (9CI) (CA INDEX NAME)



IT **108-70-3**, 1,3,5-Trichlorobenzene
(regioselective preparation of meta-substituted anilines by palladium-free amination of aryl chlorides)
RN 108-70-3 HCAPLUS
CN Benzene, 1,3,5-trichloro- (8CI, 9CI) (CA INDEX NAME)



CC 27-11 (Heterocyclic Compounds (One Hetero Atom))
IT 90-04-0, 2-Methoxyaniline 92-67-1, 4-Phenylaniline 98-16-8, 3-(Trifluoromethyl)aniline **348-54-9**, 2-Fluoroaniline **371-40-4**, 4-Fluoroaniline 610-49-1, 1-Aminoanthracene 28469-92-3, 2,6-Dichlorostyrene
(preparation of 2,3-dihydroindoles and indoles by palladium-free amination-cyclization or amination of chlorostyrenes)
IT 95-50-1, 1,2-Dichlorobenzene 95-72-7 100-46-9, Benzylamine, reactions 100-61-8, N-Methylaniline, reactions 103-49-1, Dibenzylamine **108-70-3**, 1,3,5-Trichlorobenzene 108-90-7, Chlorobenzene, reactions 109-89-7, Diethylamine, reactions 110-89-4, Piperidine, reactions 110-91-8, Morpholine, reactions 111-92-2, Di-n-butylamine 541-73-1, 1,3-Dichlorobenzene 766-51-8, 1-Chloro-2-methoxybenzene 2845-89-8, 1-Chloro-3-methoxybenzene 54423-01-7
(regioselective preparation of meta-substituted anilines by palladium-free amination of aryl chlorides)
REFERENCE COUNT: 69 THERE ARE 69 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L64 ANSWER 8 OF 55 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:824207 HCAPLUS Full-text
DOCUMENT NUMBER: 133:362614
TITLE: Preparation of substituted anilines by

hydrogenolysis of the corresponding phenylhydrazines.

INVENTOR(S): Ancel, Jean-Erick; Perrin-Janet, Gilles; Leroy, Pierre

PATENT ASSIGNEE(S): Aventis CropScience SA, Fr.

SOURCE: PCT Int. Appl., 12 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

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PRIORITY APPLN. INFO.:			GB 1999-11180	A
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OTHER SOURCE(S): CASREACT 133:362614; MARPAT 133:362614

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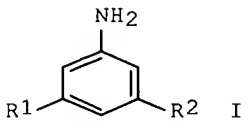


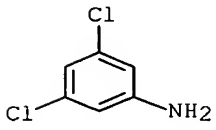
I

AB Title compds. (I; R1, R2 = halo) were prepared by hydrogenolysis of the corresponding phenylhydrazines in the presence of a metal or a metal compound under reducing conditions. Thus, 3,5-dichlorophenylhydrazine was heated with wet Raney Ni in MeOH at 60° for 2 h to give 100% 3,5-dichloroaniline.

IT **626-43-7P**, 3,5-Dichloroaniline
(preparation of substituted anilines by hydrogenolysis of the corresponding phenylhydrazines)

RN 626-43-7 HCAPLUS

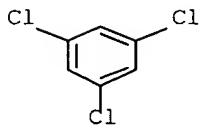
CN Benzenamine, 3,5-dichloro- (9CI) (CA INDEX NAME)



IT **108-70-3**, 1,3,5-Trichlorobenzene
(preparation of substituted anilines by hydrogenolysis of the corresponding phenylhydrazines)

RN 108-70-3 HCAPLUS

CN Benzene, 1,3,5-trichloro- (8CI, 9CI) (CA INDEX NAME)



IC ICM C07C209-42
ICS C07C211-52
CC 25-4 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 5
IT **626-43-7P**, 3,5-Dichloroaniline
(preparation of substituted anilines by hydrogenolysis of the corresponding phenylhydrazines)
IT **108-70-3**, 1,3,5-Trichlorobenzene 7440-02-0, Nickel, reactions
(preparation of substituted anilines by hydrogenolysis of the corresponding phenylhydrazines)
REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L64 ANSWER 9 OF 55 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:699230 HCAPLUS Full-text
DOCUMENT NUMBER: 133:252148
TITLE: Preparation of 3,5-difluoroaniline from 1,3,5-trichlorobenzene via fluorination and amination.
INVENTOR(S): Cherney, Lee I.; Mettille, Francis J.
PATENT ASSIGNEE(S): BASF Corporation, USA
SOURCE: U.S., 12 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6127577	A	20001003	US 2000-500368 <--	2000 0208
CA 2398650	AA	20010816	CA 2001-2398650 <--	2001 0201
WO 2001058846	A1	20010816	WO 2001-EP1079 <--	2001 0201

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW,

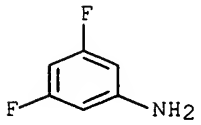
MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL,
TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM,
AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE,
CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,
PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR,
NE, SN, TD, TG

EP 1254103	A1	20021106	EP 2001-919251	2001 0201 <--
EP 1254103	B1	20040526		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
BR 2001008169	A	20030225	BR 2001-8169	2001 0201 <--
JP 2003534242	T2	20031118	JP 2001-558398	2001 0201 <--
AT 267796	E	20040615	AT 2001-919251	2001 0201 <--
PRIORITY APPLN. INFO.:			US 2000-500368 A	2000 0208 <--
			WO 2001-EP1079 W	2001 0201 <--

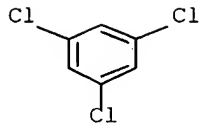
OTHER SOURCE(S): CASREACT 133:252148

AB 3,5-Difluoroaniline was prepared by fluorination of 1,3,5-trichlorobenzene to make 1,3,5-trifluorobenzene and amination of the latter. Thus, 1,3,5-trifluorobenzene and NH3 were autoclaved in diethylene glycol at 230° and 960 psig for 10 h to give 95% conversion to 3,5-difluoroaniline. Apparatus diagrams are given.

IT **372-39-4P**, 3,5-Difluoroaniline
(preparation of 3,5-difluoroaniline from 1,3,5-trichlorobenzene via fluorination and amination)
RN 372-39-4 HCAPLUS
CN Benzenamine, 3,5-difluoro- (9CI) (CA INDEX NAME)

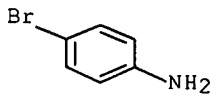


IT **108-70-3**, 1,3,5-Trichlorobenzene
(preparation of 3,5-difluoroaniline from 1,3,5-trichlorobenzene via fluorination and amination)
RN 108-70-3 HCAPLUS
CN Benzene, 1,3,5-trichloro- (8CI, 9CI) (CA INDEX NAME)

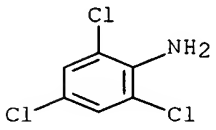


IC ICM C07C209-10
INCL 564407000
CC 25-3 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 45, 47
IT **372-39-4P**, 3,5-Difluoroaniline
(preparation of 3,5-difluoroaniline from 1,3,5-trichlorobenzene via fluorination and amination)
IT **108-70-3**, 1,3,5-Trichlorobenzene
(preparation of 3,5-difluoroaniline from 1,3,5-trichlorobenzene via fluorination and amination)
REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

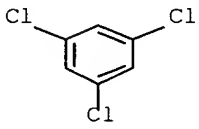
L64 ANSWER 10 OF 55 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:498573 HCAPLUS Full-text
DOCUMENT NUMBER: 133:252090
TITLE: A mild one-pot deamination of aromatic amines bearing electron-withdrawing groups. Calcium hypophosphite as a dediazonation reagent in nonaqueous media
AUTHOR(S): Mitsuhashi, H.; Kawakami, T.; Suzuki, H.
CORPORATE SOURCE: School of Science, Department of Chemistry, Kwansei Gakuin University, Uegahara, Nishinomiya, 662-8501, Japan
SOURCE: Tetrahedron Letters (**2000**), 41(29), 5567-5569
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 133:252090
AB Diazotization of aromatic amines with NO2 in MeCN at -20°, followed by treatment with Ca(H2PO2)2 in the presence of MeOH and catalytic amts. of FeSO4 at room temperature results in the reductive removal of the amino group, giving the corresponding arenes in moderate to good yield.
IT **106-40-1**, 4-Bromoaniline **634-93-5**, 2,4,6-Trichloroaniline
(deamination of aromatic amines with calcium hypophosphite as dediazonation reagent in nonaq. media)
RN 106-40-1 HCAPLUS
CN Benzenamine, 4-bromo- (9CI) (CA INDEX NAME)



RN 634-93-5 HCAPLUS
CN Benzenamine, 2,4,6-trichloro- (9CI) (CA INDEX NAME)



IT **108-70-3P**, 1,3,5-Trichlorobenzene
(deamination of aromatic amines with calcium hypophosphite as dediazonation reagent in nonaq. media)
RN 108-70-3 HCAPLUS
CN Benzene, 1,3,5-trichloro- (8CI, 9CI) (CA INDEX NAME)



CC 25-6 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
IT 97-02-9, 2,4-Dinitroaniline 100-01-6, 4-Nitroaniline, reactions **106-40-1**, 4-Bromoaniline 108-69-0, 3,5-Dimethylaniline 121-87-9, 2-Chloro-4-nitroaniline 603-83-8, 2-Methyl-3-nitroaniline **634-93-5**, 2,4,6-Trichloroaniline 17420-30-3, 2-Cyano-4-nitroaniline
(deamination of aromatic amines with calcium hypophosphite as dediazonation reagent in nonaq. media)
IT 88-72-2P, 1-Methyl-2-nitrobenzene 98-95-3P, Nitrobenzene, preparation 99-65-0P, 1,3-Dinitrobenzene 108-38-3P, 1,3-Dimethylbenzene, preparation **108-70-3P**, 1,3,5-Trichlorobenzene 108-86-1P, Bromobenzene, preparation 121-73-3P, 1-Chloro-3-nitrobenzene 619-24-9P, 3-Nitrobenzonitrile
(deamination of aromatic amines with calcium hypophosphite as dediazonation reagent in nonaq. media)
REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L64 ANSWER 11 OF 55 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:505666 HCAPLUS Full-text
DOCUMENT NUMBER: 131:144417
TITLE: N-(Hetero)aryl-3,4-(cyclo)alkoxybenzamides and analogs useful as tumor necrosis factor and c-AMP phosphodiesterase inhibitors
INVENTOR(S): Fenton, Garry; Morley, Andrew David; Palfreyman, Malcolm Norman; Ratcliffe, Andrew James; Harp, Brian William; Thurairatnam, Sukanthini; Vacher, Bernard Yvon Jack; Ashton,

Michael John; Cook, David Charles; Hills, Susan Jacqueline; McFarlane, Ian Michael; Vicker, Nigel

PATENT ASSIGNEE(S): Rhone-Poulenc Rorer Ltd., UK

SOURCE: U.S., 48 pp.
CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5935978	A	19990810	US 1993-98178	1993 0728
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ZA 9200547	A	19930503	ZA 1992-547	1992 0127
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WO 9212961	A1	19920806	WO 1992-GB153	1992 0128
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RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, MC, NL, SE				
AU 9211881	A1	19920827	AU 1992-11881	1992 0128
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AU 664694	B2	19951130		
EP 569414	A1	19931118	EP 1992-903462	1992 0128
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R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
JP 06504782	T2	19940602	JP 1992-503280	1992 0128
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PL 169994	B1	19960930	PL 1992-300142	1992 0128
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CZ 281894	B6	19970312	CZ 1993-1528	1992 0128
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NO 9302701	A	19930921	NO 1993-2701	1993 0727
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ZA 9305448	A	19940519	ZA 1993-5448	1993 0728
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ES 2227519	T3	20050401	ES 1993-917937	1993

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FI 9500375	A	19950127	FI 1995-375	
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US 5679696	A	19971021	US 1995-484805	
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US 5698711	A	19971216	US 1995-487377	
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US 5840724	A	19981124	US 1997-881888	
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US 6255326	B1	20010703	US 1999-239075	
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US 6096768	A	20000801	US 1999-301877	
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PRIORITY APPLN. INFO.:			GB 1991-1777	A
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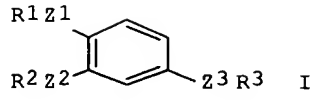
OTHER SOURCE(S): MARPAT 131:144417

GI



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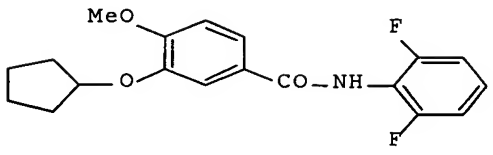


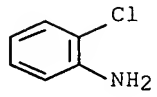
II

AB Title compds. (I) [R1 = lower alkyl; R2 = (un)substituted cycloalkyl, (un)substituted cycloalkenyl, (un)substituted or oxidized cyclothioalkyl, or (un)substituted or oxidized cyclothioalkenyl; R3 = (un)substituted (hetero)aryl; Z, Z1, Z2 = independently O or S; Z3 = C(:Z)NH] and their N-oxides and salts were prepared for pharmaceutical use as tumor necrosis factor and cAMP phosphodiesterase inhibitors. Thus, 3-cyclopentyloxy-4-methoxybenzoyl chloride (preparation given) in CH2Cl2 was added dropwise to 2,6-difluoroaniline in triethylamine and CH2Cl2 and refluxed for 4 h to yield N-(2,6-difluorophenyl)-3-cyclopentyloxy- 4-methoxybenzamide (II). Compds. of the invention were tested for inhibitory effects on PDE activity and eosinophil superoxide generation, effects on tracheal smooth muscle contractility, in vivo bronchodilator actions and antigen(ovalbamin)-induced eosinophilia, in vitro inhibitory effects on TNF-α release by human monocytes, and inhibitory effects on antigen-induced bronchoconstriction in conscious guinea-pigs and serum TNF-α levels in LPS-challenged mice. Compds. showed 10,000-fold to 50-fold more selectivity for cAMP phosphodiesterase IV than cyclic nucleotide phosphodiesterase types I, III, or V and have IC50 values ranging from 0.1 nM to 40 μM for PDE activity. At concns. from 5x10-9M to 10-5M, preferably 5x10-9 to 10-7, compds. produced about 50% relaxation of guinea-pig tracheal strips. When administered at EDs of 4 to 1000 μg/kg, preferably 4 to 50 μg/kg, compds. produced 30% to 90% decrease in bronchospasm without any significant effect on blood pressure. At oral doses of 1 to 50 mg/kg, preferably 1 to 10 mg/kg, and inhaled doses of 4 to 1000 μg/kg,

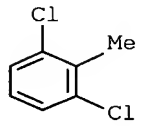
preferably 4 to 50 μg/kg, compds. inhibited by at least 50% ovalbumin-induced eosinophilia in guinea-pigs. Compds. produced 50% inhibition of LPS-induced TNF-α release from human PBMs at concns. of 10-9M to 10-6M, preferably 10-9M to 10-8 M. At doses of 1 to 1000 μg/kg (i.t.), preferably 1 to 20 μg/kg (i.t.), compds. inhibited antigen-induced bronchoconstriction by up to 80%. Compds. inhibited LPS-induced serum TNF-α at doses of 10 to 10,000 μg/kg, preferably 10 to 250 μg/kg. Compds. showed very low mammalian toxicity levels. Twenty-one compns. of the title compds. for gelatin capsules or dry powder inhalers were also prepared

IT **95-51-2**, 2-Chloroaniline **118-69-4**, 2,6-Dichlorotoluene **5509-65-9**, 2,6-Difluoroaniline
(reactant; preparation of N-(hetero)aryl 3,4-(cyclo)alkoxybenzamides and analogs useful as tumor necrosis factor and c-AMP phosphodiesterase inhibitors)

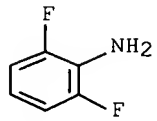
RN 95-51-2 HCAPLUS
CN Benzenamine, 2-chloro- (9CI) (CA INDEX NAME)



RN 118-69-4 HCAPLUS
CN Benzene, 1,3-dichloro-2-methyl- (9CI) (CA INDEX NAME)



RN 5509-65-9 HCAPLUS
CN Benzenamine, 2,6-difluoro- (9CI) (CA INDEX NAME)



IC A61K031-44; C07D213-75
INCL 514352000
CC 25-19 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 1, 63

IT 75-26-3, 2-Bromopropane **95-51-2**, 2-Chloroaniline
96-40-2, 3-Chloro-1-cyclopentene 100-09-4, p-Anisic acid
106-94-5 108-85-0, Cyclohexyl bromide 108-89-4, 4-Picoline
109-65-9, 1-Butyl bromide **118-69-4**, 2,6-Dichlorotoluene

137-43-9, Cyclopentyl bromide 139-85-5, 3,4-Dihydroxybenzaldehyde 356-80-9, 1-Chloromethyl-2,2,3,3-tetrafluorocyclobutane 497-36-9 504-24-5, 4-Aminopyridine 531-37-3, 2-Methoxyphenyl benzoate 619-14-7, 3-Hydroxy-4-nitrobenzoic acid 621-59-0, 3-Hydroxy-4-methoxybenzaldehyde 693-58-3, 1-Bromononane 721-09-5, Methyl 3-amino-4-trifluoromethoxybenzoate 937-14-4, 3-Chloroperbenzoic acid 1687-53-2, 5-Amino-2-methoxyphenol 2457-47-8, 3,5-Dichloropyridine 3334-05-2, 3-Hydroxythiophane 3814-30-0, Cyclopentylmethyl bromide 4659-45-4, 2,6-Dichlorobenzoyl chloride **5509-65-9**, 2,6-Difluoroaniline 6702-50-7, Methyl 3-hydroxy-4-methoxybenzoate 6921-34-2, Benzylmagnesium chloride 7051-34-5, Cyclopropylmethyl bromide 13378-44-4 14719-83-6, Methyl 4-chloro-3-nitrobenzoate 18063-02-0, 2,6-Difluorobenzoyl chloride 20511-15-3, 4-Chloro-3-pyridylamine 20973-90-4, 2,6-Dichlorophenylacetaldehyde 31329-64-3, 4-Amino-3,5-dimethylisoxazole 33216-52-3, 3,4,5-Trichloropyridine 36367-85-8, 4-(p-Toluenesulfonoxy)-1-cyclopentene 36779-79-0 38222-83-2, 2,6-Bis(tert-butyl)-4-methylpyridine 39920-37-1, 2,6-Dichlorophenyl isocyanate 61277-90-5 72093-04-0, 3-Chloro-4-methylpyridine 84539-34-4, 4-Amino-3,5-dibromopyridine 105252-95-7, 4-Amino-2,3,5-trifluoropyridine 107724-65-2, 4-Bromo-2-hydroxythioanisole 131408-41-8 135637-42-2 135637-44-4 155997-09-4 159782-23-7, 3-(2-Fluorocyclopentyloxy)-4-methoxybenzoyl chloride 159783-11-6, 3-Cyclopentylthio-4-methoxybenzoyl chloride 159783-15-0, 3-Cyclopentyloxy-4,N-dimethoxy-N-methylbenzamide 159783-38-7, 3-Isopropoxy-4-(methylthio)benzoyl chloride 159783-44-5, 4-Bromo-2-prop-2-yloxythioanisole 159783-47-8, 3-(3-Methyl-2-butenyloxy)-4-methoxybenzoic acid 159783-48-9, 3-Isopropoxy-4-difluoromethoxybenzoic acid 159783-54-7 159783-55-8 159783-73-0 159783-76-3 159783-79-6, 2,6-Dichlorobenzyltriphenylphosphonium bromide 159783-80-9, 2,6-Difluorobenzyltriphenylphosphonium bromide 159783-82-1, 4-(Difluoromethoxy)-3-isopropoxybenzaldehyde 166742-05-8 171802-54-3 192376-90-2, 3-Cyclopentyloxy-4-methoxyphenol 236422-25-6 236422-26-7 236422-32-5
(reactant; preparation of N-(hetero)aryl 3,4-(cyclo)alkoxybenzamides and analogs useful as tumor necrosis factor and c-AMP phosphodiesterase inhibitors)

REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

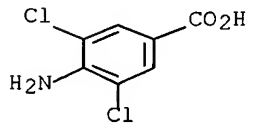
L64 ANSWER 12 OF 55 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1998:736128 HCAPLUS Full-text
DOCUMENT NUMBER: 130:68120
TITLE: Oxidative Chlorination, Desulfonation, or Decarboxylation To Synthesize Pharmaceutical Intermediates: 2,6-Dichlorotoluene, 2,6-Dichloroaniline, and 2,6-Dichlorophenol
AUTHOR(S): Mukhopadhyay, S.; Chandalia, S. B.
CORPORATE SOURCE: Department of Chemical Technology, University of Mumbai, Matunga Mumbai, 400 019, India
SOURCE: Organic Process Research & Development (**1999**), 3(1), 10-16
CODEN: OPRDFK; ISSN: 1083-6160
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB An alternative manufacturing process scheme was developed for 2,6-dichlorotoluene, 2,6-dichloroaniline, and 2,6-dichlorophenol, involving oxidative chlorination of the p-substituted benzoic or benzenesulfonic acid followed by decarboxylation or desulfonation. Oxidative chlorination of p-methylbenzenesulfonic acid, p-methylbenzoic acid, p-aminobenzoic acid, and p-hydroxybenzoic acid, and subsequent desulfonation or decarboxylation gave a 60-75% yield of the desired products.

IT **56961-25-2P**, 4-Amino-3,5-dichlorobenzoic acid
(intermediate; in preparation of dichloroaniline)

RN 56961-25-2 HCAPLUS

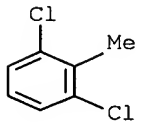
CN Benzoic acid, 4-amino-3,5-dichloro- (6CI, 9CI) (CA INDEX NAME)



IT **118-69-4P**, 2,6-Dichlorotoluene **608-31-1P**, 2,6-Dichloroaniline
(preparation by oxidative chlorination of acid derivative)

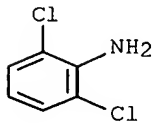
RN 118-69-4 HCAPLUS

CN Benzene, 1,3-dichloro-2-methyl- (9CI) (CA INDEX NAME)



RN 608-31-1 HCAPLUS

CN Benzenamine, 2,6-dichloro- (9CI) (CA INDEX NAME)



CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)

IT **56961-25-2P**, 4-Amino-3,5-dichlorobenzoic acid
(intermediate; in preparation of dichloroaniline)

IT 87-65-0P, 2,6-Dichlorophenol **118-69-4P**, 2,6-Dichlorotoluene **608-31-1P**, 2,6-Dichloroaniline
(preparation by oxidative chlorination of acid derivative)

REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L64 ANSWER 13 OF 55 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1998:585961 HCAPLUS Full-text
DOCUMENT NUMBER: 129:189110
TITLE: Preparation of 3,5-difluoraniline from 3,5-difluorochlorobenzene.
INVENTOR(S): Pfirmann, Ralf; Krause, Stefan
PATENT ASSIGNEE(S): Clariant G.m.b.H., Germany
SOURCE: Ger., 8 pp.
CODEN: GWXXAW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19720341	C1	19980827	DE 1997-19720341 <--	1997 0515
EP 878461	A2	19981118	EP 1998-107389 <--	1998 0423
EP 878461	A3	19990901		
EP 878461	B1	20020410		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 10330334	A2	19981215	JP 1998-130504 <--	1998 0513
US 5965775	A	19991012	US 1998-78012 <--	1998 0513
PRIORITY APPLN. INFO.:			DE 1997-19720341 A <--	1997 0515

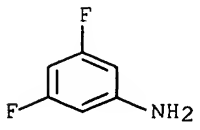
OTHER SOURCE(S): CASREACT 129:189110

AB 3,5-Difluoroaniline (I) was prepared by treatment of 3,5-difluorochlorobenzene (II) with NH3 in the presence of >1 of Cu, Fe, Co, Ni, Cr, Mo, or Zn at 100-250°. Thus, 0.05 mol II was autoclaved with 0.5 mol 25% aqueous NH3, 0.015 mol CuCl, and 0.015 mol Cu at 150° for 24 h to give 78% I.

IT **372-39-4P**, 3,5-Difluoroaniline
(preparation of 3,5-difluoraniline from 3,5-difluorochlorobenzene)

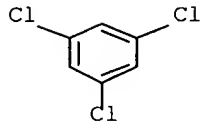
RN 372-39-4 HCAPLUS

CN Benzenamine, 3,5-difluoro- (9CI) (CA INDEX NAME)

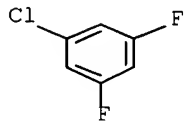


IT **108-70-3**, 1,3,5-Trichlorobenzene

(preparation of 3,5-difluoraniline from 3,5-difluorochlorobenzene)
RN 108-70-3 HCAPLUS
CN Benzene, 1,3,5-trichloro- (8CI, 9CI) (CA INDEX NAME)



IT **1435-43-4P**, 3,5-Difluorochlorobenzene
(preparation of 3,5-difluoraniline from 3,5-difluorochlorobenzene)
RN 1435-43-4 HCAPLUS
CN Benzene, 1-chloro-3,5-difluoro- (7CI, 8CI, 9CI) (CA INDEX NAME)



IC ICM C07C211-52
ICS C07C209-10
CC 25-4 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
IT **372-39-4P**, 3,5-Difluoroaniline
(preparation of 3,5-difluoraniline from 3,5-difluorochlorobenzene)
IT **108-70-3**, 1,3,5-Trichlorobenzene
(preparation of 3,5-difluoraniline from 3,5-difluorochlorobenzene)
IT **1435-43-4P**, 3,5-Difluorochlorobenzene
(preparation of 3,5-difluoraniline from 3,5-difluorochlorobenzene)
REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L64 ANSWER 14 OF 55 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1998:239214 HCAPLUS Full-text
DOCUMENT NUMBER: 128:282833
TITLE: Preparation of 4-phenyl-2-thiazoleamines as corticotropin releasing factor antagonists
INVENTOR(S): Fontaine, Evelyne; Gully, Danielle; Roger, Pierre; Wermuth, Camille Georges
PATENT ASSIGNEE(S): Sanofi, Fr.; Fontaine, Evelyne; Gully, Danielle; Roger, Pierre; Wermuth, Camille Georges
SOURCE: PCT Int. Appl., 62 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

WO 9815543 A1 19980416 WO 1997-FR1788
1997
1007
<--
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG

FR 2754258 A1 19980410 FR 1996-12256
1996
1008
<--

FR 2754258 B1 19981231

CA 2267154 AA 19980416 CA 1997-2267154
1997
1007
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AU 9746270 A1 19980505 AU 1997-46270
1997
1007
<--

EP 934290 A1 19990811 EP 1997-944937
1997
1007
<--

EP 934290 B1 20020417
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI

BR 9712507 A 19991221 BR 1997-12507
1997
1007
<--

JP 2000504039 T2 20000404 JP 1998-517261
1997
1007
<--

JP 3290998 B2 20020610

AT 216375 E 20020515 AT 1997-944937
1997
1007
<--

ES 2174298 T3 20021101 ES 1997-944937
1997
1007
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US 6344470 B1 20020205 US 1999-269516
1999
0402
<--

NO 9901637 A 19990607 NO 1999-1637
1999
0407
<--

NO 312725 B1 20020624

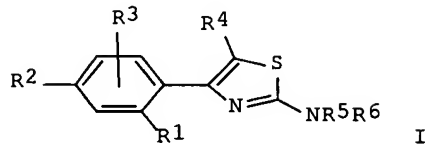
MX 9903241	A	20000731	MX 1999-3241	1999 0407 <--
US 2002137740	A1	20020926	US 2001-998949	2001 1115 <--

PRIORITY APPLN. INFO.:

FR 1996-12256	A	1996 1008 <--
WO 1997-FR1788	W	1997 1007 <--
US 1999-269516	A1	1999 0402 <--

OTHER SOURCE(S): MARPAT 128:282833

GI



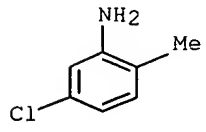
I

AB Title compds. [I; R1,R2 = halo, (hydroxy)alkyl, alkoxy(carbonyl), CONH2, etc.; R3 = H and groups cited for R1; R4 = halo, alkyl, CH2OH, CHO; R5 = (hydroxy)alkyl, alkenyl, alkynyl, etc.; R6 = (un)substituted Ph, heteroaryl, etc.] were prepared as corticotropin releasing factor receptor antagonists (no data). Thus, 2,5-MeClC6H3NHCSNH2 was cyclocondensed with 2,4-Cl(MeO)C6H3COCHMeBr (preparation each given) to give I (R1 = Cl, R2 = OMe, R3 = H, R4 = Me, R6 = C6H3MeCl-2,5)(II; R5 = H) which was N-alkylated by PrI to give II (R5 = Pr).

IT **95-79-4**, 5-Chloro-2-methylaniline **108-70-3**, 1,3,5-Trichlorobenzene **554-00-7**, 2,4-Dichloroaniline
(preparation of 4-phenyl-2-thiazoleamines as corticotropin releasing factor antagonists)

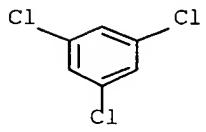
RN 95-79-4 HCAPLUS

CN Benzenamine, 5-chloro-2-methyl- (9CI) (CA INDEX NAME)

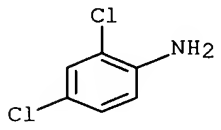


RN 108-70-3 HCAPLUS

CN Benzene, 1,3,5-trichloro- (8CI, 9CI) (CA INDEX NAME)



RN 554-00-7 HCAPLUS
CN Benzenamine, 2,4-dichloro- (9CI) (CA INDEX NAME)



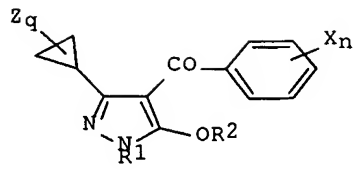
IC ICM C07D277-42
ICS C07D417-12; A61K031-425
CC 28-7 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 2
IT 79-03-8, Propionyl chloride 79-09-4, Propanoic acid, reactions **95-79-4**, 5-Chloro-2-methylaniline 98-88-4, Benzoyl chloride 106-94-5, 1-Bromopropane 106-96-7, Propargyl bromide **108-70-3**, 1,3,5-Trichlorobenzene 110-91-8, Morpholine, reactions **554-00-7**, 2,4-Dichloroaniline 1068-55-9, Isopropylmagnesium chloride 1730-48-9, 7-Methoxy-1,2,3,4-tetrahydronaphthalene 1813-33-8, 2-Chloro-4-trifluoromethylbenzonitrile 3002-94-6, Cyclopropyl lithium 7693-52-9, 4-Bromo-2-nitrophenol 16419-60-6, 2-Methylphenylboronic acid 24812-90-6, Methyl 3-amino-4-methoxybenzoate 50868-73-0, 2-Methoxy-6-methylaniline 103175-61-7, 2-Bromo-1-(2,4-dichlorophenyl)-1-propanone 188120-55-0 205758-37-8 205758-38-9 205758-39-0
(preparation of 4-phenyl-2-thiazoleamines as corticotropin releasing factor antagonists)
REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L64 ANSWER 15 OF 55 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1997:740214 HCAPLUS Full-text
DOCUMENT NUMBER: 128:13263
TITLE: Preparation of 1-alkyl-4-benzoyl-3-cyclopropyl-5-hydroxypyrazoles and derivatives as herbicides.
INVENTOR(S): Murai, Shigeo; Kikugawa, Hiroshi; Nakayama, Hitoshi; Sano, Makiko; Isogai, Akihiko
PATENT ASSIGNEE(S): Ishihara Sangyo Kaisha Ltd., Japan
SOURCE: PCT Int. Appl., 148 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9741106	A1	19971106	WO 1997-JP1457	19970425
			<--	
W: BG, CA, CN, CZ, HU, KR, MX, PL, RO, RU, SI, SK, US, YU RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
JP 10109976	A2	19980428	JP 1997-110389	19970411
			<--	
ZA 9703559	A	19971119	ZA 1997-3559	19970424
			<--	
CA 2252451	AA	19971106	CA 1997-2252451	19970425
			<--	
EP 900205	A1	19990310	EP 1997-919701	19970425
			<--	
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
CN 1216535	A	19990512	CN 1997-194093	19970425
			<--	
BR 9701948	A	19990112	BR 1997-1948	19970428
			<--	
US 5998334	A	19991207	US 1998-147191	19981026
			<--	
PRIORITY APPLN. INFO.:			JP 1996-130879 A	19960426
			<--	
			JP 1996-227767 A	19960809
			<--	
			WO 1997-JP1457 W	19970425
			<--	

OTHER SOURCE(S): MARPAT 128:13263
GI



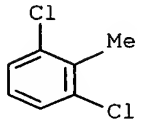
I

AB Title compds. [I; R1 = alkyl; R2 = H, Me, AR3, (substituted) Ph, pyridyl, phenylallyl; A = SO2, CO, CHR6, CHR7CO; R3 = (substituted), alkyl, alkenyl, alkynyl, alkoxy, Ph, cyano, dialkylamino; R6, R7 = H, alkyl; X = H, halo, alkyl, haloalkyl, alkoxy, alkylthio, alkylsulfinyl, alkylsulfonyl, NO2, alkoxycarbonyl, SO2NR8R9, NR10SO2R11, CH2SOR12 OSO2mR13; R8-R13 = alkyl; Z = alkyl; q = 0-5; n = 1-5; q = 0-2; provided that when q ≥2, a plurality of Z may be the same or different, and when n ≥2, a plurality of X may be the same or different], were prepared Thus, MeNHNH2 was refluxed with tert-Bu 3-cyclopropyl-3-oxopropionate in THF to give 3-cyclopropyl-5- hydroxy-1-methylpyrazole. This was stirred with aqueous Na2CO3 and 4-trifluoromethyl-2-methylthiobenzoyl chloride (prepared in situ) in PhMe to give 3-cyclopropyl-1-methyl-5-pyrazolyl-4-trifluoromethyl- 2-methylthiobenzoate. This was converted to 3-cyclopropyl-4-(4- trifluoromethyl-2-methylsulfonylbenzoyl)-5-hydroxy-1- methylpyrazole. The latter at 125 g/ha postemergent gave 100% control of Xanthium strumarium.

IT **118-69-4**, 2,6-Dichlorotoluene
(preparation of 1-alkyl-4-benzoyl-3-cyclopropyl-5-hydroxypyrazoles and derivs. as herbicides)

RN 118-69-4 HCAPLUS

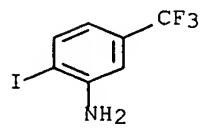
CN Benzene, 1,3-dichloro-2-methyl- (9CI) (CA INDEX NAME)



IT **105202-02-6P**
(preparation of 1-alkyl-4-benzoyl-3-cyclopropyl-5-hydroxypyrazoles and derivs. as herbicides)

RN 105202-02-6 HCAPLUS

CN Benzenamine, 2-iodo-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)



IC ICM C07D231-20
ICS C07D401-12; A01N043-56

CC 28-8 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 5

IT 60-34-4, Methylhydrazine 78-88-6, 2,3-Dichloropropene 89-75-8, 2,4-Dichlorobenzoyl chloride **118-69-4**, 2,6-Dichlorotoluene 302-01-2, Hydrazine, reactions 400-97-5 134302-07-1, tert-Butyl 3-cyclopropyl-3-oxopropionate 142994-05-6
(preparation of 1-alkyl-4-benzoyl-3-cyclopropyl-5-hydroxypyrazoles and derivs. as herbicides)

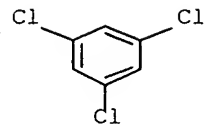
IT **105202-02-6P** 199125-21-8P 199125-22-9P 199125-23-0P 199125-24-1P 199125-25-2P 199125-26-3P 199125-27-4P 199125-28-5P 199125-29-6P 199125-30-9P 199125-31-0P 199125-32-1P 199125-33-2P 199125-34-3P 199125-35-4P 199125-36-5P
(preparation of 1-alkyl-4-benzoyl-3-cyclopropyl-5-hydroxypyrazoles and derivs. as herbicides)

L64 ANSWER 16 OF 55 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1997:697238 HCAPLUS Full-text
DOCUMENT NUMBER: 128:3490
TITLE: Fluorinated biphenyls from aromatic arylation with pentafluorobenzenediazonium and related cations. Competition between arylation and azo coupling
AUTHOR(S): Kosynkin, Dmitry; Bockman, T. Michael; Kochi, Jay K.
CORPORATE SOURCE: Dep. Chemistry, Univ. Houston, Houston, TX, 77204-5641, USA
SOURCE: Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (**1997**), (10), 2003-2012
CODEN: JCPKBH; ISSN: 0300-9580
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 128:3490

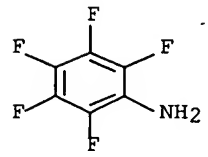
AB High yields of the mixed perfluorinated biaryls (C6F5-Ar) are obtained by the catalytic dediazoniation of the pentafluorobenzenediazonium salt (C6F5N2+ BF4-) in acetonitrile solns. containing various aromatic substrates (ArH) together with small amts. of iodide salts. Activated (electron-rich) as well as deactivated (electron-poor) arenes are successfully pentafluorophenylated by this method. The arylation is distinct from the azo coupling of the same substrates, which takes place in the absence of the iodide catalyst and yields the corresponding diazene (C6F5N=N-Ar) as product. The catalytic role of iodide, and the isomeric product distributions obtained with this procedure indicate that the arylation proceeds via the pentafluorophenyl radical in an efficient homolytic chain process. Since azo coupling involves electrophilic aromatic substitution of electron-rich ArH by C6H5N2+, the two competing pathways are distinct and do not have reactive intermediates in common.

IT **108-70-3**, 1,3,5-Trichlorobenzene **771-60-8**, Pentafluoroaniline
(preparation, arylation and azo coupling of pentafluorobenzenediazonium and related cations)

RN 108-70-3 HCAPLUS
CN Benzene, 1,3,5-trichloro- (8CI, 9CI) (CA INDEX NAME)



RN 771-60-8 HCAPLUS
CN Benzenamine, 2,3,4,5,6-pentafluoro- (9CI) (CA INDEX NAME)



CC 25-3 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
IT 71-43-2, Benzene, reactions 91-16-7 91-20-3, Naphthalene, reactions 94-09-7, Ethyl 4-aminobenzoate 95-47-6, o-Xylene, reactions 98-06-6, tert-Butylbenzene 98-82-8, Isopropylbenzene 98-95-3, Nitrobenzene, reactions 99-09-2, 3-Nitroaniline 100-01-6, 4-Nitroaniline, reactions 100-66-3, Anisole, reactions 100-84-5, 3-Methylanisole 106-42-3, p-Xylene, reactions 106-46-7, p-Dichlorobenzene 108-38-3, reactions 108-67-8, Mesitylene, reactions **108-70-3**, 1,3,5-Trichlorobenzene 108-88-3, reactions 108-90-7, Chlorobenzene, reactions 150-78-7, p-Dimethoxybenzene 151-10-0 328-74-5, 3,5-Bis(trifluoromethyl)aniline 618-87-1, 3,5-Dinitroaniline 700-12-9, 1,2,3,4,5-Pentamethylbenzene **771-60-8**, Pentafluoroaniline 42122-73-6, Diethyl 5-aminoisophthalate 190671-96-6
(preparation, arylation and azo coupling of pentafluorobenzenediazonium and related cations)
REFERENCE COUNT: 74 THERE ARE 74 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L64 ANSWER 17 OF 55 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1997:314628 HCAPLUS Full-text
DOCUMENT NUMBER: 127:50482
TITLE: Epoxidation of alkenes under liquid-liquid biphasic conditions: synthesis and catalytic activity of Mn(III)-tetraarylporphyrins bearing perfluoroalkyl tails
AUTHOR(S): Pozzi, Gianluca; Colombani, Ida; Miglioli, Massimo; Montanari, Fernando; Quici, Silvio
CORPORATE SOURCE: Centro CNR and Dipartimento di Chimica Organica e Industriale dell'Universita, Milan, I-20133, Italy
SOURCE: Tetrahedron (**1997**), 53(17), 6145-6162
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal

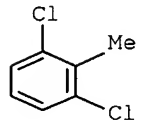
LANGUAGE: English
OTHER SOURCE(S): CASREACT 127:50482

AB Four tetraarylporphyrins bearing one n-C8F17 chain on each meso-aryl group have been synthesized. The Mn(III)-complexes of these new compds. were used as catalysts in alkene epoxidns. carried out under aqueous-organic biphasic conditions. High epoxide yields were obtained with catalysts in which, along with perfluoroalkyl chains, bulky substituents were present at appropriate positions. The expected general enhancement of stability and catalytic activity due to the electron-withdrawing effect of n-C8F17 substituents was not observed However, one of the Mn(III)-complexes was found to be an exceptionally active catalyst for NaOCl promoted epoxidn. of poorly reactive linear α-alkenes.

IT **118-69-4**, 2,6-Dichlorotoluene
(epoxidn. of alkenes under liquid-liquid biphasic conditions)

RN 118-69-4 HCAPLUS

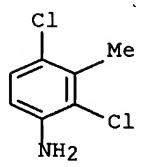
CN Benzene, 1,3-dichloro-2-methyl- (9CI) (CA INDEX NAME)



IT **19853-79-3P**
(epoxidn. of alkenes under liquid-liquid biphasic conditions)

RN 19853-79-3 HCAPLUS

CN Benzenamine, 2,4-dichloro-3-methyl- (9CI) (CA INDEX NAME)



CC 27-2 (Heterocyclic Compounds (One Hetero Atom))

IT 109-97-7, Pyrrole 112-41-4, 1-Dodecene **118-69-4**, 2,6-Dichlorotoluene 498-66-8, Bicyclo[2.2.1]hept-2-ene 507-63-1, Perfluorooctyl iodide 591-49-1, 1-Methylcyclohexene 618-91-7, Methyl m-iodobenzoate 619-44-3, Methyl p-iodobenzoate 629-73-2, 1-Hexadecene 872-05-9, 1-Decene 931-88-4, Cyclooctene 1073-67-2, 4-Chlorostyrene 18516-37-5, 2-Methyl-1-undecene 177167-51-0
(epoxidn. of alkenes under liquid-liquid biphasic conditions)

IT **19853-79-3P** 29682-46-0P 80791-11-3P 80791-12-4P 134641-34-2P 134641-35-3P 163114-33-8P 190722-63-5P 190722-64-6P 190722-65-7P 190722-66-8P 190722-69-1P 190722-70-4P 190722-75-9P 190722-77-1P 190722-78-2P 190722-79-3P 190722-80-6P 190722-81-7P 190722-82-8P 190722-83-9P
(epoxidn. of alkenes under liquid-liquid biphasic conditions)

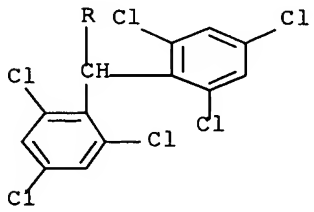
REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE

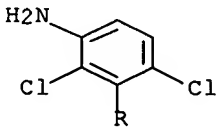
IN THE RE FORMAT

L64 ANSWER 18 OF 55 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1996:309983 HCAPLUS Full-text
DOCUMENT NUMBER: 125:85903
TITLE: (2,6-Dichlorophenyl)bis(2,4,6-trichlorophenyl)methyl radical. Synthesis, Magnetic Behavior and Crystal Structure
AUTHOR(S): Carilla, Jose; Fajari, Lluis; Julia, Luis; Sane, Joan; Rius, Jordi
CORPORATE SOURCE: Dep. Mater. Org. Halogenats, CSIC, Barcelona, 08034, Spain
SOURCE: Tetrahedron (**1996**), 52(20), 7013-7024
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

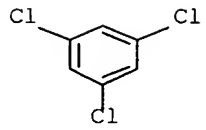
AB (2,6-Dichlorophenyl)bis(2,4,6-trichlorophenyl)methyl radical (I) was prepared through a reaction sequence of five stages via four new intermediate compds. . Assignment of the structures of these compds. was confirmed by 1H NMR spectra. The new persistent radical I was characterized by EPR spectra and magnetic susceptibility measurements. The x-ray structural anal. of I shows that it adopts a propeller-like conformation with the Ph rings twisted around their bonds to trivalent carbon. Magnetic susceptibility of I is characteristic of a paramagnet with a weak antiferromagnetic interaction at low temps. (Weiss constant, θ = -1.8 K).

IT **178421-50-6P**
(intermediate in preparation of (dichlorophenyl)bis(trichlorophenyl) methyl radical)
RN 178421-50-6 HCAPLUS
CN Benzenamine, 3-[bis(2,4,6-trichlorophenyl)methyl]-2,4-dichloro- (9CI) (CA INDEX NAME)



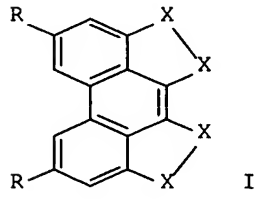


IT **108-70-3**, 1,3,5-Trichlorobenzene
(reactant in preparation of (dichlorophenyl)bis(trichlorophenyl)methyl radical)
RN 108-70-3 HCAPLUS
CN Benzene, 1,3,5-trichloro- (8CI, 9CI) (CA INDEX NAME)



CC 22-3 (Physical Organic Chemistry)
Section cross-reference(s): 75
IT 178421-48-2P 178421-49-3P **178421-50-6P** 178421-51-7P
(intermediate in preparation of (dichlorophenyl)bis(trichlorophenyl) methyl radical)
IT 81-19-6, α,α,2,6-Tetrachlorotoluene **108-70-3**
, 1,3,5-Trichlorobenzene
(reactant in preparation of (dichlorophenyl)bis(trichlorophenyl)meth yl radical)

L64 ANSWER 19 OF 55 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:900537 HCAPLUS Full-text
DOCUMENT NUMBER: 124:117461
TITLE: Syntheses, structures and properties of phenanthro[1,10-cd:8,9-c'd']bis[1,2]-dithiole and -diselenole and their methyl and methylthio derivatives as novel electron donors
AUTHOR(S): Takimiya, Kazuo; Shibata, Youji; Ohnishi, Akiko; Aso, Yoshio; Otsubo, Tetsuo; Ogura, Fumio
CORPORATE SOURCE: Dep. Applied Chem., Hiroshima Univ., Higashi-Hiroshima, 739, Japan
SOURCE: Journal of Materials Chemistry (**1995**), 5(10), 1539-47
CODEN: JMACEP; ISSN: 0959-9428
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

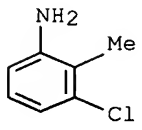
AB Tetrathio- and tetraseleno-phenanthrenes, as well as their di-Me and bis(methylthio) derivs. I (X = S, Se; R = H, Me, MeS) were synthesized as the 1st examples of novel electron donors of the peri-dichalcogen-bridged polyphene type. X-ray analyses revealed that these compds. have planar heterocyclic structures similar to that of perylene, in the crystal, the mols. are stacked in columns with strong interactions between the heteroatoms in adjacent columns, which produces a two- or three-dimensional interactive

network of the mol. components. Cyclic voltammetry studies indicated that these compds. have somewhat weaker electron-donating abilities than do their anthracene counterparts bearing structural resemblances. Although only tetraselenophenanthrene gave a conductive charge-transfer complex with 7,7,8,8-tetracyanoquinodimethane (TCNQ), they all formed complexes with stronger electron acceptors, 2,3,5,6-tetrafluoro- TCNQ (TCNQF4) and 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (DDQ), giving rare examples of conductive materials containing TCNQF4 and DDQ. They formed a variety of radical cation salts, which are also highly conductive.

IT **87-60-5 118-69-4**, 2,6-Dichlorotoluene
(syntheses and properties of phenanthrobisdithioles and -diselenoles as novel electron donors)

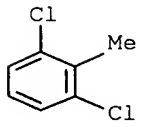
RN 87-60-5 HCAPLUS

CN Benzenamine, 3-chloro-2-methyl- (9CI) (CA INDEX NAME)



RN 118-69-4 HCAPLUS

CN Benzene, 1,3-dichloro-2-methyl- (9CI) (CA INDEX NAME)



CC 29-8 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 72, 75, 76

IT **87-60-5** 89-98-5 **118-69-4**, 2,6-Dichlorotoluene
(syntheses and properties of phenanthrobisdithioles and -diselenoles as novel electron donors)

L64 ANSWER 20 OF 55 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:725628 HCAPLUS Full-text

DOCUMENT NUMBER: 123:198203

TITLE: Physical, spectral and chromatographic properties of all 209 individual PCB congeners

AUTHOR(S): Bolgar, Michael; Cunningham, James; Cooper, Russell; Kozloski, Richard; Hubball, Jack

CORPORATE SOURCE: AccuStandard Inc., New Haven, CT, 06511, USA

SOURCE: Chemosphere (**1995**), 31(2), 2687-705
CODEN: CMSHAF; ISSN: 0045-6535

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

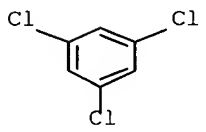
AB Phys., spectral and chromatog. data for all 209 individual PCB congeners is presented. The individual congeners were synthesized and then isolated and purified. Through the use of two capillary GC columns: 40% octadecyl/15% Ph

Me siloxane and 50% Ph Me siloxane, it was possible to sep. 201 PCB congeners with only 4 unresolved pairs.

IT **108-70-3**, 1,3,5-Trichlorobenzene **626-43-7**, 3,5-Dichloroaniline
(preparation and phys., spectral, and chromatog. properties of all PCB congeners)

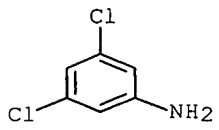
RN 108-70-3 HCAPLUS

CN Benzene, 1,3,5-trichloro- (8CI, 9CI) (CA INDEX NAME)



RN 626-43-7 HCAPLUS

CN Benzenamine, 3,5-dichloro- (9CI) (CA INDEX NAME)



CC 22-13 (Physical Organic Chemistry)

IT 71-43-2, Benzene, reactions 87-61-6, 1,2,3-Trichlorobenzene 95-50-1, 1,2-Dichlorobenzene 95-51-2, 2-Chloroaniline 95-76-1, 3,4-Dichloroaniline 95-82-9, 2,5-Dichloroaniline 95-94-3, 1,2,4,5-Tetrachlorobenzene 106-46-7, 1,4-Dichlorobenzene 106-47-8, 4-Chloroaniline, reactions 108-42-9, 3-Chloroaniline **108-70-3**, 1,3,5-Trichlorobenzene 108-90-7, Chlorobenzene, reactions 120-82-1, 1,2,4-Trichlorobenzene 541-73-1, 1,3-Dichlorobenzene 554-00-7, 2,4-Dichloroaniline 608-27-5, 2,3-Dichloroaniline 608-31-1, 2,6-Dichloroaniline 608-93-5, Pentachlorobenzene **626-43-7**, 3,5-Dichloroaniline 634-66-2, 1,2,3,4-Tetrachlorobenzene 634-67-3, 2,3,4-Trichloroaniline 634-83-3, 2,3,4,5-Tetrachloroaniline 634-90-2, 1,2,3,5-Tetrachlorobenzene 634-91-3, 3,4,5-Trichloroaniline 634-93-5, 2,4,6-Trichloroaniline 636-30-6, 2,4,5-Trichloroaniline 654-36-4, 2,3,4,6-Tetrachloroaniline 3481-20-7, 2,3,5,6-Tetrachloroaniline 18487-39-3, 2,3,5-Trichloroaniline 88963-39-7, 2,3,6-Trichloroaniline
(preparation and phys., spectral, and chromatog. properties of all PCB congeners)

L64 ANSWER 21 OF 55 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1993:603121 HCAPLUS Full-text

DOCUMENT NUMBER: 119:203121

TITLE: Preparation of 3,5-dichloroaniline from trichlorobenzene

INVENTOR(S): Fujino, Toshihiro; Sato, Haruyo

PATENT ASSIGNEE(S): Toray Industries, Japan

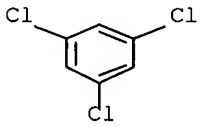
SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 05194330	A2	19930803	JP 1992-8738	19920121

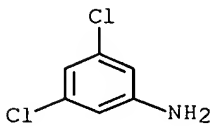
PRIORITY APPLN. INFO.: JP 1992-8738 19920121
OTHER SOURCE(S): CASREACT 119:203121

AB 3,5-Dichloroaniline (I) is prepared by treating 1,3,5- trichlorobenzene (II) with NH3 in presence of Cu catalysts and N-methyl-ε-caprolactam (III) or 2-pyrrolidone. A mixture of II, III, CuCl, and liquid NH3 was heated at 200° for 6 h to give I with 59.6% conversion and 85.1% selectivity.

IT **108-70-3**, 1,3,5-Trichlorobenzene
(amination of, by ammonia, solvents for)
RN 108-70-3 HCAPLUS
CN Benzene, 1,3,5-trichloro- (8CI, 9CI) (CA INDEX NAME)



IT **626-43-7P**, 3,5-Dichloroaniline
(preparation of, from trichlorobenzene)
RN 626-43-7 HCAPLUS
CN Benzenamine, 3,5-dichloro- (9CI) (CA INDEX NAME)

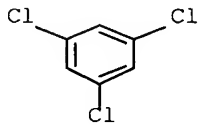


IC ICM C07C211-52
ICS B01J031-28; C07C209-10
ICA C07B061-00
CC 25-4 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
IT **108-70-3**, 1,3,5-Trichlorobenzene
(amination of, by ammonia, solvents for)
IT **626-43-7P**, 3,5-Dichloroaniline
(preparation of, from trichlorobenzene)

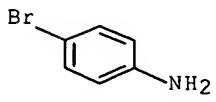
L64 ANSWER 22 OF 55 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1993:436232 HCAPLUS Full-text
DOCUMENT NUMBER: 119:36232
TITLE: Heterogeneous catalysts for use in anodic electrosyntheses and electrodestruction of organic compounds in aqueous surfactant systems
AUTHOR(S): Franklin, Thomas C.; Darlington, Jerald; Nnodimele, Remi; Duty, Robert C.
CORPORATE SOURCE: Dep. Chem., Baylor Univ., Waco, TX, 76798, USA
SOURCE: Electrochem. Colloids Dispersions, [Symp. Electrochem. Microheterog. Fluids] (**1992**), 319-29. Editor(s): Mackay, Raymond A.; Texter, John. VCH: New York, N.Y. CODEN: 58XTAL
DOCUMENT TYPE: Conference
LANGUAGE: English

AB Results of studies on the development of solid insol. catalysts for use in electrooxidns. of organic compds. in aqueous cationic surfactant suspensions are presented. Coulometric studies indicate that 1 can electrooxidize lower-valent oxides to produce Cu(III) oxide, Mn(III) and Mn(IV) oxides, and Ba superoxide. These higher oxides are able to oxidize several compds. The primary reaction produced no observed product other than carbonate and the soluble halide ion. However, di-Et sulfide was oxidized by Cu(III) oxide to produce the sulfoxide. Substituted bromobenzenes with the Br oriented into the aqueous phase of the suspension were readily destroyed, while those that had the Br oriented into the micelle were readily attacked. Also a Ba peroxide catalyzed system can be used as a fuel cell, generating small amts. of electricity while destroying the compound

IT **108-70-3**, 1,3,5-Trichlorobenzene
(destruction of, in battery, barium peroxide in relation to)
RN 108-70-3 HCAPLUS
CN Benzene, 1,3,5-trichloro- (8CI, 9CI) (CA INDEX NAME)

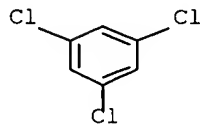


IT **106-40-1**, p-Bromoaniline
(electrochem. oxidation and destruction of, on platinum in sodium nitrate solution containing tetrabutylammonium hydroxide and barium peroxide)
RN 106-40-1 HCAPLUS
CN Benzenamine, 4-bromo- (9CI) (CA INDEX NAME)

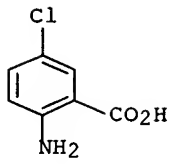


CC 72-2 (Electrochemistry)
Section cross-reference(s): 22, 52
IT **108-70-3**, 1,3,5-Trichlorobenzene
(destruction of, in battery, barium peroxide in relation to)
IT 88-65-3, o-Bromobenzoic acid 106-38-7, p-Bromotoluene
106-40-1, p-Bromoaniline 586-76-5, p-Bromobenzoic acid
(electrochem. oxidation and destruction of, on platinum in sodium nitrate solution containing tetrabutylammonium hydroxide and barium peroxide)

L64 ANSWER 23 OF 55 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1992:577869 HCAPLUS Full-text
DOCUMENT NUMBER: 117:177869
TITLE: Gibbs free energy of formation of halogenated aromatic compounds and their potential role as electron acceptors in anaerobic environments
AUTHOR(S): Dolfing, Jan; Harrison, B. Keith
CORPORATE SOURCE: Dep. Biochem., Univ. Groningen, Groningen, 9747 AG, Neth.
SOURCE: Environmental Science and Technology (**1992**), 26(11), 2213-18
CODEN: ESTHAG; ISSN: 0013-936X
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The Gibbs free energies of formation of various classes of halogenated aromatic compds. were estimated by Benson's method. The data were used to evaluate the potential of these compds. to serve as electron acceptors in anaerobic environments. The results indicate that for (chloro) benzenes, benzoates, and phenols, the redox potentials of the couples Ar-X/Ar-H are 266-478 mV. This implies that microorganisms can potentially conserve energy for growth by routing electrons in the form of H2 from anaerobic environments to halogenated aromatic compds. as electron acceptors. This theor. prediction was corroborated for 3-chlorobenzoate. The existence of enrichment cultures, obtained from anaerobic sediments and sewage sludges, that dechlorinate other halogenated aromatic compds. suggests the existence of more microorganisms that can benefit from the use of halogenated aromatic compds. as electron acceptors.
IT **108-70-3P**, 1,3,5-Trichlorobenzene **635-21-2P**
(formation of, Gibbs free energy of, biodegrdn. and water pollution in relation to)
RN 108-70-3 HCAPLUS
CN Benzene, 1,3,5-trichloro- (8CI, 9CI) (CA INDEX NAME)



RN 635-21-2 HCAPLUS
CN Benzoic acid, 2-amino-5-chloro- (9CI) (CA INDEX NAME)



CC 61-2 (Water)
Section cross-reference(s): 10, 60, 69

IT 50-45-3P 50-73-7P 50-79-3P 50-84-0P 51-36-5P 51-39-8P 58-90-2P, 2,3,4,6-Tetrachlorophenol 65-85-0P, Benzoic acid, preparation 71-43-2DP, Benzene, chloro derivs. 87-61-6P, 1,2,3-Trichlorobenzene 87-65-0P, 2,6-Dichlorophenol 87-86-5P, Pentachlorophenol 88-06-2P, 2,4,6-Trichlorophenol 95-50-1P, 1,2-Dichlorobenzene 95-57-8P, 2-Chlorophenol 95-77-2P, 3,4-Dichlorophenol 95-94-3P, 1,2,4,5-Tetrachlorobenzene 95-95-4P, 2,4,5-Trichlorophenol 106-46-7P, 1,4-Dichlorobenzene 106-48-9P, 4-Chlorophenol 108-43-0P, 3-Chlorophenol **108-70-3P**, 1,3,5-Trichlorobenzene 108-90-7P, Monochlorobenzene, preparation 108-95-2DP, Phenol, chloro derivs. 118-74-1P, Hexachlorobenzene 118-91-2P 120-82-1P, 1,2,4-Trichlorobenzene 120-83-2P, 2,4-Dichlorophenol 321-14-2P 541-73-1P, 1,3-Dichlorobenzene 576-24-9P, 2,3-Dichlorophenol 583-78-8P, 2,5-Dichlorophenol 591-35-5P, 3,5-Dichlorophenol 608-93-5P, Pentachlorobenzene 609-19-8P, 3,4,5-Trichlorophenol 618-51-9P 634-66-2P, 1,2,3,4-Tetrachlorobenzene 634-90-2P, 1,2,3,5-Tetrachlorobenzene **635-21-2P** 933-75-5P, 2,3,6-Trichlorophenol 933-78-8P, 2,3,5-Trichlorophenol 935-95-5P, 2,3,5,6-Tetrachlorophenol 2365-27-7P, 4-Fluorobenzoate 2365-28-8P, 3-Fluorobenzoate 4641-33-2P, 4-Chlorobenzoate 4901-51-3P, 2,3,4,5-Tetrachlorophenol 5377-71-9P, 4-Iodobenzoate 7499-06-1P 15950-66-0P, 2,3,4-Trichlorophenol 16426-56-5P, 2-Fluorobenzoate 16449-27-7P, 4-Bromobenzoate 16887-60-8P, 3-Chlorobenzoate 16887-61-9P, 3-Bromobenzoate 16887-76-6P, 2-Bromobenzoate 16887-77-7P, 2-Iodobenzoate 45939-19-3P 95467-67-7P, 2,6-Dichlorobenzoate
(formation of, Gibbs free energy of, biodegrdn. and water pollution in relation to)

L64 ANSWER 24 OF 55 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1992:469498 HCAPLUS Full-text
DOCUMENT NUMBER: 117:69498
TITLE: One step conversion of anilines to aryl halides using sodium nitrite and halotrimethylsilane
AUTHOR(S): Lee, Jong Gun; Cha, Hee Tae
CORPORATE SOURCE: Dep. Chem., Pusan Natl. Univ., Pusan, 609-735, S. Korea
SOURCE: Tetrahedron Letters (**1992**), 33(22), 3167-8
CODEN: TELEAY; ISSN: 0040-4039.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 117:69498

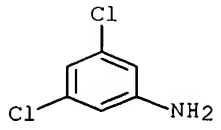
AB Anilines were easily diazotized and efficiently converted to aryl halides in a one-pot reaction using sodium nitrite and halotrimethylsilane in carbon tetrachloride. Halotrimethylsilanes are used for both generating the

nitrosonium donor from sodium nitrite, and halogen substitution of the diazonium group.

IT **626-43-7**, 3,5-Dichloroaniline
(one step conversion of, to aryl halide by sodium nitrite-halotrimethylsilane)

RN 626-43-7 HCAPLUS

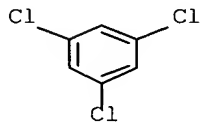
CN Benzenamine, 3,5-dichloro- (9CI) (CA INDEX NAME)



IT **108-70-3P**, 1,3,5-Trichlorobenzene
(preparation of, by reaction of aniline derivative with sodium nitrite-halotrimethylsilane)

RN 108-70-3 HCAPLUS

CN Benzene, 1,3,5-trichloro- (8CI, 9CI) (CA INDEX NAME)



CC 25-3 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

IT 95-51-2, o-Chloroaniline 95-53-4, o-Toluidine, reactions 97-02-9, 2,4-Dinitroaniline 108-69-0, 3,5-Dimethylaniline 134-32-7, 1-Aminonaphthalene 536-90-3, m-Anisidine 540-37-4, p-Iodoaniline 615-36-1, o-Bromoaniline **626-43-7**, 3,5-Dichloroaniline 873-74-5, p-Aminobenzonitrile
(one step conversion of, to aryl halide by sodium nitrite-halotrimethylsilane)

IT 95-49-8P, o-Chlorotoluene 97-00-7P, 2,4-Dinitrochlorobenzene **108-70-3P**, 1,3,5-Trichlorobenzene 556-96-7P, 3,5-Dimethylbromobenzene 615-41-8P, o-Chloroiodobenzene 623-03-0P, p-Chlorobenzonitrile 624-38-4P 694-80-4P, o-Bromochlorobenzene 766-85-8P, m-Iodoanisole
(preparation of, by reaction of aniline derivative with sodium nitrite-halotrimethylsilane)

L64 ANSWER 25 OF 55 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1991:655780 HCAPLUS Full-text

DOCUMENT NUMBER: 115:255780

TITLE: Process for the preparation of 2,6-difluoroaniline and intermediates

INVENTOR(S): Pews, R. Garth; Gall, James A.

PATENT ASSIGNEE(S): DowElanco, USA

SOURCE: U.S., 6 pp.
CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

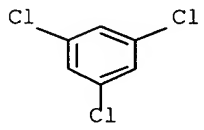
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5041674	A	19910820	US 1990-537975	19900614

PRIORITY APPLN. INFO.: US 1990-537975 19900614

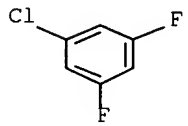
OTHER SOURCE(S): CASREACT 115:255780

AB A process for the preparation of 2,6-F2C6H3NH2 (I) comprises chlorination of 3,5-F2C6H3Cl (II) to give 4,6-difluoro-1,2,3- trichlorobenzene which is nitrated and reduced to give I. Thus, chlorination of II with chlorine gas in the presence of SbCl3 as catalyst in CH2Cl2 followed by nitration with 90% HNO3 gave a mixture of 3% 4,6-difluoro-1,2,3,5-tetrachlorobenzene, 18% 2,4-difluoro-3,5,6-trichloronitrobenzene, and 76% 2,6-difluoro-3,4,5-trichloronitrobenzene. Hydrogenation of this mixture in a Hastelloy C pressure reactor in the presence of Pd/charcoal/hydrogen in MeOH gave 89% I and 11% 2,4-F2C6H3NH2.

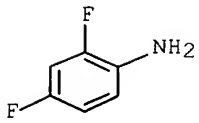
IT **108-70-3**, 1,3,5-Trichlorobenzene
(fluorination of, with potassium fluoride)
RN 108-70-3 HCAPLUS
CN Benzene, 1,3,5-trichloro- (8CI, 9CI) (CA INDEX NAME)



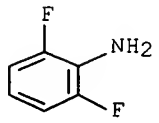
IT **1435-43-4P**, 1-Chloro-3,5-difluorobenzene
(preparation and chlorination of)
RN 1435-43-4 HCAPLUS
CN Benzene, 1-chloro-3,5-difluoro- (7CI, 8CI, 9CI) (CA INDEX NAME)



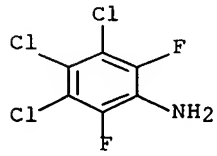
IT **367-25-9P**, 2,4-Difluoroaniline **5509-65-9P**, 2,6-Difluoroaniline **136272-34-9P**, 2,6-Difluoro-3,4,5-trichloroaniline
(preparation of)
RN 367-25-9 HCAPLUS
CN Benzenamine, 2,4-difluoro- (9CI) (CA INDEX NAME)



RN 5509-65-9 HCAPLUS
CN Benzenamine, 2,6-difluoro- (9CI) (CA INDEX NAME)



RN 136272-34-9 HCAPLUS
CN Benzenamine, 3,4,5-trichloro-2,6-difluoro- (9CI) (CA INDEX NAME)



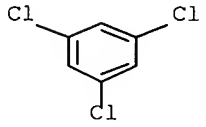
IC ICM C07C211-46
ICS C07C209-22
INCL 564442000
CC 25-4 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
IT **108-70-3**, 1,3,5-Trichlorobenzene
(fluorination of, with potassium fluoride)
IT **1435-43-4P**, 1-Chloro-3,5-difluorobenzene
(preparation and chlorination of)
IT **367-25-9P**, 2,4-Difluoroaniline 372-38-3P,
1,3,5-Trifluorobenzene 1198-56-7P, 4,6-Difluoro-1,2,3,5-tetrachlorobenzene 1435-46-7P, 1,3-Dichloro-5-fluorobenzene
5509-65-9P, 2,6-Difluoroaniline **136272-34-9P**,
2,6-Difluoro-3,4,5-trichloroaniline
(preparation of)

L64 ANSWER 26 OF 55 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1991:558603 HCAPLUS Full-text
DOCUMENT NUMBER: 115:158603
TITLE: Aromatic fluorine chemistry. Part 4. Preparation of 2,6-difluoroaniline
AUTHOR(S): Pews, R. G.; Gall, J. A.
CORPORATE SOURCE: Cent. Res. Lab., Dow Chem. Co., Midland, MI, 48674, USA
SOURCE: Journal of Fluorine Chemistry (**1991**), 52(3), 307-16

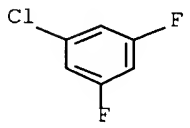
CODEN: JFLCAR; ISSN: 0022-1139
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The preparation of 2,6-difluoroaniline from 1,3,5-trichlorobenzene is described. 1-Chloro-3,5-difluorobenzene prepared via F exchange on 1,3,5-trichlorobenzene is dichlorinated and nitrated in a single reactor to a mixture of trichlorodifluoronitrobenzenes. The latter are reduced by catalytic hydrogenation to give a .apprx.4:1 mixture of 2,6- and 2,4-difluoroaniline.

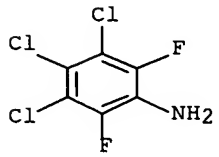
IT **108-70-3**, 1,3,5-Trichlorobenzene
(fluorination of, by halogen exchange with potassium fluoride)
RN 108-70-3 HCAPLUS
CN Benzene, 1,3,5-trichloro- (8CI, 9CI) (CA INDEX NAME)



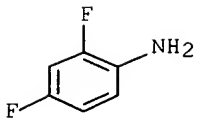
IT **1435-43-4P**, 1-Chloro-3,5-difluorobenzene
(preparation and nitration of)
RN 1435-43-4 HCAPLUS
CN Benzene, 1-chloro-3,5-difluoro- (7CI, 8CI, 9CI) (CA INDEX NAME)



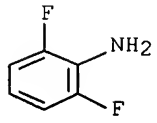
IT **136272-34-9P**
(preparation of)
RN 136272-34-9 HCAPLUS
CN Benzenamine, 3,4,5-trichloro-2,6-difluoro- (9CI) (CA INDEX NAME)



IT **367-25-9P**, 2,4-Difluoroaniline **5509-65-9P**, 2,6-Difluoroaniline
(preparation of, from trichlorobenzene)
RN 367-25-9 HCAPLUS
CN Benzenamine, 2,4-difluoro- (9CI) (CA INDEX NAME)

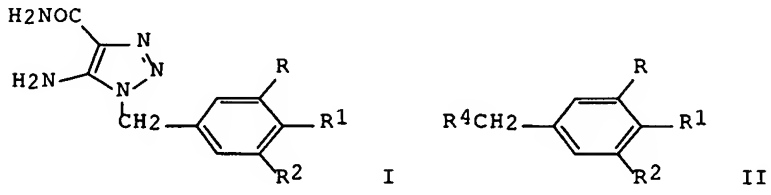


RN 5509-65-9 HCAPLUS
CN Benzenamine, 2,6-difluoro- (9CI) (CA INDEX NAME)



CC 25-4 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
IT **108-70-3**, 1,3,5-Trichlorobenzene
(fluorination of, by halogen exchange with potassium fluoride)
IT 1198-56-7P **1435-43-4P**, 1-Chloro-3,5-difluorobenzene
13656-67-2P 43061-38-7P 136313-38-7P
(preparation and nitration of)
IT **136272-34-9P**
(preparation of)
IT **367-25-9P**, 2,4-Difluoroaniline **5509-65-9P**,
2,6-Difluoroaniline
(preparation of, from trichlorobenzene)

L64 ANSWER 27 OF 55 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1991:536007 HCAPLUS Full-text
DOCUMENT NUMBER: 115:136007
TITLE: Benzylated 1,2,3-triazoles as anticoccidiostats
AUTHOR(S): Bochis, Richard J.; Chabala, John C.; Harris, Ellwood; Peterson, Louis H.; Barash, Louis; Beattie, Thomas; Brown, Jeannette E.; Graham, Donald W.; Waksmunski, Frank S.; et al.
CORPORATE SOURCE: Mercke Sharp and Dohme Res. Lab., Rahway, NJ, 07065-0900, USA
SOURCE: Journal of Medicinal Chemistry (**1991**), 34(9), 2843-52
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



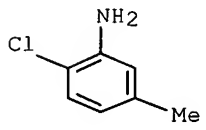
I

II

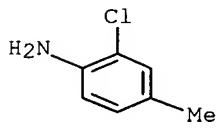
AB Substituted aminocarbamoyltriazoles I (R = Cl, H, COC6H4Cl-4; R1 = COC6H4R3, COPh, H, Cl, R3 = 4-Cl, 4-F, 4-cyano, 4-CO2Me, 4-CCl:CCl2, 4-Br, 4-iodo; R1 = COC6H3Cl2-3,4, COC6H3Cl2-2,6, etc.; R2 = H, Cl, F, Br) were prepared and evaluated in vivo for anticoccidial activity. Thus, N-alkylation of 5-amino-4-carbamoyl-1,2,3-triazole with benzene derivs. II (R4 = Br) gave I. Cyclization of II (R4 = N3) with 2-cyanoacetamide also gave I. I (R = R2 = Cl, R1 = COC6H4Cl-4) is a highly effective coccidiostat. An increase in activity was observed when the CO of the benzophenone moiety is flanked by halogens as in I (R = R2 = Cl, R1 = COC6H4Cl-4; R = R2 = Cl, R1 = COPh).

IT **95-81-8 615-65-6**
(bromination of)

RN 95-81-8 HCAPLUS
CN Benzenamine, 2-chloro-5-methyl- (9CI) (CA INDEX NAME)

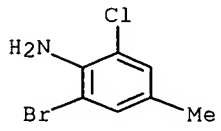


RN 615-65-6 HCAPLUS
CN Benzenamine, 2-chloro-4-methyl- (9CI) (CA INDEX NAME)



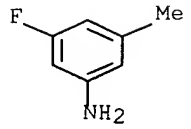
IT **135340-78-2P**
(preparation and cyanation of)

RN 135340-78-2 HCAPLUS
CN Benzenamine, 2-bromo-6-chloro-4-methyl- (9CI) (CA INDEX NAME)

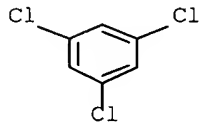


IT **52215-41-5P**
(preparation and diazotization-chlorination of)

RN 52215-41-5 HCAPLUS
CN Benzenamine, 3-fluoro-5-methyl- (9CI) (CA INDEX NAME)

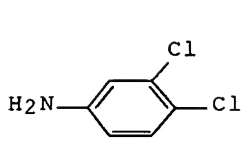


IT **108-70-3P**
(preparation, lithiation, carboxylation, and acylation of)
RN 108-70-3 HCAPLUS
CN Benzene, 1,3,5-trichloro- (8CI, 9CI) (CA INDEX NAME)

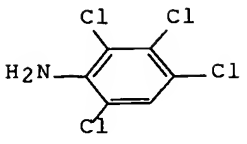


CC 28-10 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1
IT **95-81-8** 106-43-4 108-88-3, reactions **615-65-6**
(bromination of)
IT **135340-78-2P**
(preparation and cyanation of)
IT **52215-41-5P**
(preparation and diazotization-chlorination of)
IT **108-70-3P** 93857-90-0P
(preparation, lithiation, carboxylation, and acylation of)

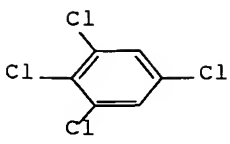
L64 ANSWER 28 OF 55 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1991:163624 HCAPLUS Full-text
DOCUMENT NUMBER: 114:163624
TITLE: Halogenation using quaternary ammonium polyhalides, XXIX. Chlorination of aromatic amines with benzyltrimethylammonium tetrachloroiodate and deamination of the chloro-substituted aromatic amines
AUTHOR(S): Kakinami, Takaaki; Noazu, Takashi; Yonemaru, Satoshi; Okamoto, Tsuyoshi; Shinmasu, Yoichi; Kajigaeshi, Shoji
CORPORATE SOURCE: Dep. Chem. Biol. Eng., Ube Tech. Coll., Ube, 755, Japan
SOURCE: Nippon Kagaku Kaishi (**1991**), (1), 44-9
CODEN: NKAKB8; ISSN: 0369-4577
DOCUMENT TYPE: Journal
LANGUAGE: Japanese
OTHER SOURCE(S): CASREACT 114:163624
GI



I



II



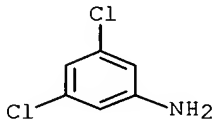
III

AB The reaction of aromatic amines, e.g., I with a calculated amount of benzyltrimethylammonium tetrachloroiodate in AcOH at room temperature or at 70° gave chloro-substituted aromatic amines, e.g., II in good yields. The reaction of the chloro-substituted aromatic amines with sodium nitrite and phosphinic acid in 18 N sulfuric acid at 0 .apprx. 5° gave the deamination products, e.g., III.

IT **626-43-7**
(chlorination of, with benzyltrimethylammonium tetrachloroiodate)

RN 626-43-7 HCAPLUS

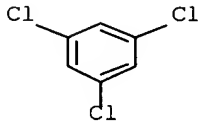
CN Benzenamine, 3,5-dichloro- (9CI) (CA INDEX NAME)



IT **108-70-3P**
(preparation of)

RN 108-70-3 HCAPLUS

CN Benzene, 1,3,5-trichloro- (8CI, 9CI) (CA INDEX NAME)



CC 25-4 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

IT 88-74-4, 2-Nitroaniline 95-51-2, 2-Chloroaniline 95-76-1 95-82-9 99-09-2, 3-Nitroaniline 99-52-5 99-55-8 100-01-6, 4-Nitroaniline, reactions 106-40-1, 4-Bromoaniline 106-47-8, 4-Chloroaniline, reactions 108-42-9, 3-Chloroaniline 118-92-3, 2-Aminobenzoic acid 150-13-0, 4-Aminobenzoic acid 536-90-3, 3-Methoxyaniline 554-00-7 591-19-5, 3-Bromoaniline 608-27-5 608-31-1 615-36-1, 2-Bromoaniline 621-33-0, 3-Ethoxyaniline **626-43-7**
(chlorination of, with benzyltrimethylammonium tetrachloroiodate)

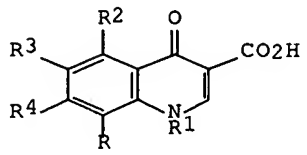
IT 87-40-1P **108-70-3P** 608-93-5P 618-62-2P 634-90-2P 16582-38-0P 18708-70-8P 19393-96-5P 19752-55-7P 23399-88-4P 89692-81-9P

(preparation of)

L64 ANSWER 29 OF 55 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1990:458966 HCAPLUS Full-text
DOCUMENT NUMBER: 113:58966
TITLE: Quinolonecarboxylic acid derivatives and their preparation as bactericides
INVENTOR(S): Masuzawa, Kuniyoshi; Suzue, Seigo; Hirai, Keiji; Ishizaki, Takayoshi
PATENT ASSIGNEE(S): Kyorin Pharmaceutical Co., Ltd., Japan
SOURCE: U.S., 11 pp. Cont.-in-part of U.S. Ser. No. 26,194, abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4894458	A	19900116	US 1988-233363 <--	19880818
JP 62215572	A2	19870922	JP 1986-59016 <--	19860317

PRIORITY APPLN. INFO.:
JP 1986-59016 A 19860317 <--
US 1987-26194 B2 19870316 <--
OTHER SOURCE(S): CASREACT 113:58966; MARPAT 113:58966
GI

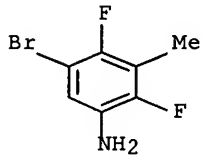


I

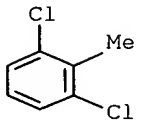
AB Title compds. I (R = alkyl; R1 = C3-6 cycloalkyl, alkyl, haloalkyl, alkenyl, hydroxyalkyl, alkylamino, Ph; R2 = H, halo, O2N, H2N; R3 = halo; R4 = halo, azetidino, pyrrolidino, piperidino, (thio)morpholino, (un)substituted (homo)piperazino, etc.) and pharmaceutically acceptable salts, are prepared I (R = Me, R1 = cyclopropyl, R2 = H, R3 = R4 = F), 3-tert-butoxycarbonylaminopyrrolidine, DBU and anhydrous MeCN were refluxed for 18 h to give I (R = Me, R1 = cyclopropyl, R2 = H, R3 = F, R4 = 3-amino-2-

pyrrolidinyl) (II). In vitro against Bacillus subtilis the min. inhibitory concentration of II was 0.025 μg/mL vs. 0.05 μg/mL for ciprofloxacin.

IT **112822-79-4P**
(preparation and reaction of, in preparation of antibacterials)
RN 112822-79-4 HCAPLUS
CN Benzenamine, 5-bromo-2,4-difluoro-3-methyl- (9CI) (CA INDEX NAME)



IT **118-69-4**, 2,6-Dichlorotoluene
(reaction of, in preparation of antibacterials)
RN 118-69-4 HCAPLUS
CN Benzene, 1,3-dichloro-2-methyl- (9CI) (CA INDEX NAME)



IC ICM C07D401-04
INCL 546156000
CC 27-17 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1
IT 51676-76-7P 112822-76-1P 112822-77-2P 112822-78-3P
112822-79-4P 112822-81-8P 112822-82-9P 112822-83-0P
112822-84-1P 112822-85-2P 112822-86-3P 112822-87-4P
112822-88-5P 112822-89-6P 112822-90-9P 112822-91-0P
112822-93-2P 112822-94-3P 112822-96-5P
(preparation and reaction of, in preparation of antibacterials)
IT 105-53-3, Diethyl malonate 110-85-0, Piperazine, reactions
118-69-4, 2,6-Dichlorotoluene 765-30-0, Cyclopropylamine
99724-19-3 107610-69-5 107610-73-1
(reaction of, in preparation of antibacterials)

L64 ANSWER 30 OF 55 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1990:440475 HCAPLUS Full-text
DOCUMENT NUMBER: 113:40475
TITLE: Antibacterial 8-methylquinolonecarboxylic acid derivative and its preparation
INVENTOR(S): Masuzawa, Kuniyasu; Suzue, Seigo; Hirai, Keiji; Ishizaki, Takayoshi
PATENT ASSIGNEE(S): Kyorin Pharmaceutical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 10 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 02019377	A2	19900123	JP 1988-168888	19880708
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PRIORITY APPLN. INFO.:			JP 1988-168888	19880708
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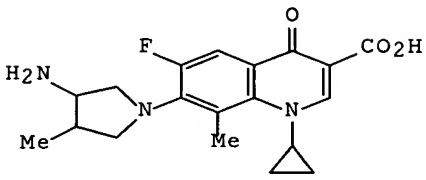
OTHER SOURCE(S): MARPAT 113:40475

GI



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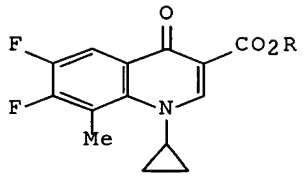


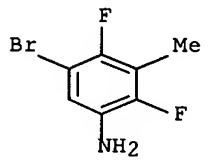
II

AB The title compound I was prepared by reaction of quinolone II (R = H, alkyl) with pyrrolidine derivs. A mixture of II (R = H) and 3,4-cis-3-tert-butoxycarbonylamino-4-methylpyrrolidine, and DBU in MeCN was stirred and refluxed for 30 h to give, after deprotection with F3CO2H, cis-I. cis-I in vitro exhibited an MIC of 0.39 μg/mL against Pseudomonas aeruginosa IFO 12689.

IT **112822-79-4P**, 5-Bromo-2,4-difluoro-3-methylaniline
(preparation and reaction of, in preparation of antibacterial agent)

RN 112822-79-4 HCAPLUS

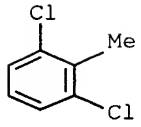
CN Benzenamine, 5-bromo-2,4-difluoro-3-methyl- (9CI) (CA INDEX NAME)



IT **118-69-4**, 2,6-Dichlorotoluene
(reaction of, in preparation of antibacterial agent)

RN 118-69-4 HCAPLUS

CN Benzene, 1,3-dichloro-2-methyl- (9CI) (CA INDEX NAME)



IC ICM C07D401-04
ICS A61K031-47
ICA C07D211-52; C07D215-56
CC 27-17 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1
IT 51676-76-7P, 2,6-Dichloro-3,5-dinitrotoluene 112822-76-1P, 2,6-Difluoro-3,5-dinitrotoluene 112822-77-2P 112822-78-3P, 3-Bromo-2,6-difluoro-5-nitrotoluene **112822-79-4P**, 5-Bromo-2,4-difluoro-3-methylaniline 112822-81-8P 112822-82-9P, 3-Bromo-2,5,6-trifluorotoluene 112822-83-0P, 2,4,5-Trifluoro-3-methylbenzonitrile 112822-84-1P 112822-85-2P, 2,4,5-Trifluoro-3-methylbenzoic acid 112822-86-3P 112822-87-4P 112822-88-5P 112822-89-6P 112822-90-9P 112822-91-0P 112822-92-1P 114174-34-4P
(preparation and reaction of, in preparation of antibacterial agent)
IT 105-53-3 **118-69-4**, 2,6-Dichlorotoluene 122-51-0, Ethyl orthoformate 765-30-0, Cyclopropylamine 107610-69-5 107610-73-1
(reaction of, in preparation of antibacterial agent)

L64 ANSWER 31 OF 55 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1989:173109 HCAPLUS Full-text
DOCUMENT NUMBER: 110:173109
TITLE: Preparation of quinolinonecarboxylates as bactericides
INVENTOR(S): Ueda, Hiraki; Miyamoto, Hisashi; Yamashita, Hiroshi; Tone, Hitoshi
PATENT ASSIGNEE(S): Otsuka Pharmaceutical Co., Ltd., Japan
SOURCE: Eur. Pat. Appl., 81 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 287951	A2	19881026	EP 1988-105959	19880414
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EP 287951	A3	19900613		
EP 287951	B1	19960703		
R: CH, DE, ES, FR, GB, IT, LI, NL, SE				
US 5563138	A	19961008	US 1988-179239	19880408
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US 5591744	A	19970107	US 1988-179300	19880408

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JP 01230558 A2 19890914 JP 1988-91121
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JP 06096557 B4 19941130
EP 565132 A2 19931013 EP 1993-107626
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EP 565132 A3 19940518
EP 565132 B1 20001025
R: CH, DE, ES, FR, GB, IT, LI, NL, SE
ES 2091180 T3 19961101 ES 1988-105959
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EP 823413 A2 19980211 EP 1997-120444
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EP 823413 A3 19981209
EP 823413 B1 20020213
R: CH, DE, ES, FR, GB, IT, LI, NL, SE
ES 2152936 T3 20010216 ES 1993-107626
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ES 2172734 T3 20021001 ES 1997-120444
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SG 97777 A1 20030820 SG 1999-120
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SG 101541 A1 20040130 SG 2002-3819
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DK 8802076 A 19881017 DK 1988-2076
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DK 170640 B1 19951120
CN 1030237 A 19890111 CN 1988-102360
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CN 1053666 B 20000621
US 5495020 A 19960227 US 1990-562034
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JP 07047575	B4	19950524		
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JP 2523092	B2	19960807		
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OTHER SOURCE(S): MARPAT 110:173109

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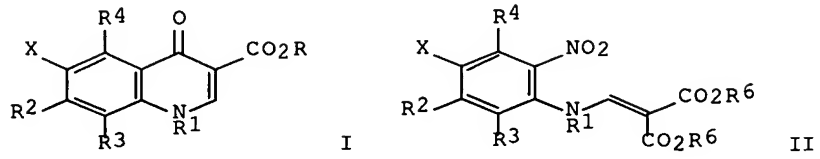
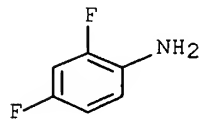


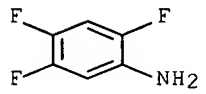
I II

AB The title compds. I [R = H, alkyl; R1 = alkenyl, thienyl; (substituted)alkyl, cyclopropyl, Ph; R2 = (substituted) 5- to 9-membered heterocyclyl; R3 = H, halo, alkyl; R4 = alkyl, halo; R1R3 = CHR5CH2O; R5 = H, alkyl; X = halo; except R3, R4 are not both = halo; when R3 = H, R4 = alkyl] are prepared, e.g., by cyclization. of anilines II (R6 = alkyl). Treatment of 3-(4-methyl-1-piperazinyl)-4-fluoro-2,5-dimethyl-6-nitro-N- cyclopropylaniline with EtOCH:CH(CO2Et)2 at 150° gave II (R1 = cyclopropyl; R2 = 4-methyl-1-piperazinyl; R3 = R4 = Me; X = F; R6 = Et), and a solution of the latter in Ac2O was heated with concentrated H2SO4 at 10-60° to give I (R = Et, R1-R4, X unchanged), which was saponified to the give the free acid (III). III had min. inhibitory concns. of 0.049 and 0.78 (no units given) against Staphylococcus aureus and S. aeruginosa, resp. An injection solution was formulated containing 200 mg III, 250 mg glucose, and H2O to make 5 mL.

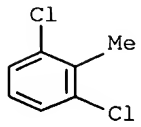
IT **367-25-9**, 2,4-Difluoroaniline
(amination by, of (ethoxymethylene)malonate)
RN 367-25-9 HCAPLUS
CN Benzenamine, 2,4-difluoro- (9CI) (CA INDEX NAME)



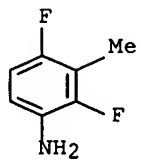
IT **367-34-0**, 2,4,5-Trifluoroaniline
(methylthiomethylation of, by di-Me sulfide)
RN 367-34-0 HCAPLUS
CN Benzenamine, 2,4,5-trifluoro- (9CI) (CA INDEX NAME)



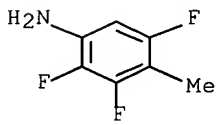
IT **118-69-4**, 2,6-Dichlorotoluene
(nitration of, in preparation of quinolinonecarboxylate bactericides)
RN 118-69-4 HCAPLUS
CN Benzene, 1,3-dichloro-2-methyl- (9CI) (CA INDEX NAME)



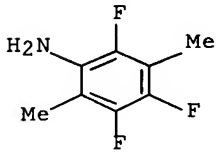
IT **76350-70-4P**, 2,4-Difluoro-3-methylaniline
119915-59-2P 119916-10-8P 119916-16-4P
119916-20-0P 119916-26-6P, 2,4,5-Trifluoro-3-methylaniline
(preparation and reaction of, in preparation of quinolinonecarboxylate bactericides)
RN 76350-70-4 HCAPLUS
CN Benzenamine, 2,4-difluoro-3-methyl- (9CI) (CA INDEX NAME)



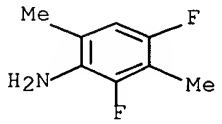
RN 119915-59-2 HCAPLUS
CN Benzenamine, 2,3,5-trifluoro-4-methyl- (9CI) (CA INDEX NAME)



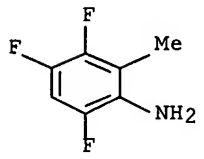
RN 119916-10-8 HCAPLUS
CN Benzenamine, 2,4,5-trifluoro-3,6-dimethyl- (9CI) (CA INDEX NAME)



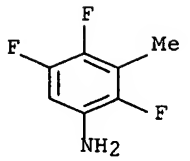
RN 119916-16-4 HCAPLUS
CN Benzenamine, 2,4-difluoro-3,6-dimethyl- (9CI) (CA INDEX NAME)



RN 119916-20-0 HCAPLUS
CN Benzenamine, 3,4,6-trifluoro-2-methyl- (9CI) (CA INDEX NAME)



RN 119916-26-6 HCAPLUS
CN Benzenamine, 2,4,5-trifluoro-3-methyl- (9CI) (CA INDEX NAME)



IC ICM C07D215-56
ICS C07D498-04; C07D401-04; C07D413-04; A61K031-47; A61K031-535
ICI C07D498-04, C07D265-00, C07D221-00
CC 27-17 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1
IT 104-94-9, 4-Methoxyaniline 141-43-5, reactions **367-25-9**, 2,4-Difluoroaniline 616-46-6, 2-Aminothiophene 870-24-6, 2-Chloroethylamine hydrochloride 2749-11-3
(amination by, of (ethoxymethylene)malonate)
IT **367-34-0**, 2,4,5-Trifluoroaniline
(methylthiomethylation of, by di-Me sulfide)
IT **118-69-4**, 2,6-Dichlorotoluene
(nitration of, in preparation of quinolinonecarboxylate bactericides)
IT 18583-89-6P 29682-46-0P, 2,6-Dichloro-3-nitrotoluene 59382-59-1P, Methyl 2-methyl-3-nitrobenzoate **76350-70-4P**, 2,4-Difluoro-3-methylaniline 79562-49-5P, 2,6-Difluoro-3-nitrotoluene 114152-18-0P, 2,3,6-Trifluoro-5-nitrotoluene 119915-41-2P, 2-Methyl-3,4,6-trifluorobenzoyl chloride 119915-42-3P 119915-43-4P 119915-44-5P 119915-45-6P 119915-46-7P 119915-47-8P 119915-48-9P 119915-49-0P 119915-50-3P 119915-51-4P 119915-52-5P 119915-53-6P 119915-54-7P 119915-55-8P 119915-56-9P 119915-57-0P 119915-58-1P, 2,3,6-Trifluoro-4-nitrotoluene **119915-59-2P** 119915-60-5P 119915-61-6P 119915-62-7P 119915-63-8P 119915-64-9P 119915-65-0P 119915-66-1P 119915-67-2P 119915-68-3P 119915-69-4P 119915-70-7P 119915-71-8P 119915-72-9P 119915-73-0P 119915-74-1P 119915-75-2P 119915-76-3P 119915-77-4P 119915-78-5P 119915-79-6P 119915-80-9P 119915-81-0P 119915-82-1P 119915-83-2P 119915-84-3P 119915-85-4P 119915-86-5P 119915-87-6P 119915-88-7P 119915-89-8P 119915-90-1P 119915-91-2P 119915-92-3P 119915-93-4P 119915-94-5P 119915-95-6P 119915-96-7P 119915-97-8P 119915-98-9P 119915-99-0P 119916-00-6P 119916-01-7P 119916-02-8P 119916-03-9P 119916-04-0P 119916-05-1P 119916-07-3P 119916-08-4P 119916-09-5P **119916-10-8P** 119916-11-9P 119916-12-0P 119916-13-1P 119916-14-2P 119916-15-3P **119916-16-4P** 119916-18-6P 119916-19-7P **119916-20-0P** 119916-21-1P, 2-Methyl-3,4,6-trifluorobenzonitrile 119916-22-2P, 2-Methyl-3,4,6-trifluorobenzoic acid 119916-24-4P 119916-25-5P, 2,3,6-Trifluorotoluene **119916-26-6P**, 2,4,5-Trifluoro-3-methylaniline 119916-27-7P 119916-28-8P 119916-29-9P 119916-30-2P 119916-31-3P 119916-32-4P 119916-33-5P 119916-34-6P 119916-35-7P 119916-36-8P 119916-37-9P 119916-38-0P 119916-39-1P 119916-40-4P 119916-41-5P 119916-42-6P 119916-43-7P 119916-44-8P
(preparation and reaction of, in preparation of quinolinonecarboxylate bactericides)

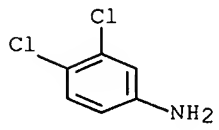
L64 ANSWER 32 OF 55 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1987:511093 HCAPLUS Full-text
DOCUMENT NUMBER: 107:111093
TITLE: Applied studies of pesticides in lysimeter plant/soil systems following application of carbon-14 labeled compounds, with particular reference to leaching behavior
AUTHOR(S): Scheunert, I.; Korte, F.; Reiml, D.
CORPORATE SOURCE: Inst. Oekol. Chem., Ges. Strahlen Umweltforsch m.b.H. Muenchen, Neuherberg, Fed. Rep. Ger.
SOURCE: Schriftenreihe des Vereins fuer Wasser-, Boden- und Lufthygiene (**1987**), 68(Grundwasserbeeinflussung Pflanzenschutzm.), 313-22
CODEN: SVWLAE; ISSN: 0300-8665
DOCUMENT TYPE: Journal
LANGUAGE: German

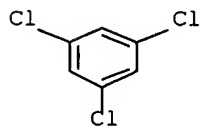
AB The fate of 14C-labeled pesticides applied to soil in field lysimeters was assessed in long-term expts. Samples of leaching water were collected at the bottom (60 cm) of the lysimeter. After application of [14C]aldrin, leached radioactivity peaked after .apprx.1.5 yr and fell to low levels after .apprx.5 yr, although some was still evident after 16.5 yr. Of several aldrin degradation products present in the soil, only dihydrochlordene dicarboxylic acid was sufficiently hydrophilic to be leached. When [14C]buturon was applied in 2 successive years, leached radioactivity peaked immediately after the 2nd application and declined steadily thereafter for 11 yr, at which time 4-chloroaniline (I) accounted for 15% of the label. When labeled I was applied to lysimeters, leached radioactivity peaked after 1.5 yr and was undetectable after 3.5 yr; 16% of the radioactivity in the leaching water was conjugated I. After application of [14C]pentachloronitrobenzene, leached label peaked after 2 yr, and was still detectable after 10 yr. After 8.5 yr, about 41% of the radioactivity was assignable to 32 chlorinated compds.

IT **95-76-1P**, 3,4-Dichloroaniline **108-70-3P**, 1,3,5-Trichlorobenzene **527-20-8P**, Pentachloroaniline **608-27-5P**, 2,3-Dichloroaniline **5930-28-9P**, 2,6-Dichloro-4-aminophenol
(pentachloronitrobenzene degradation product, leaching of, from soil)

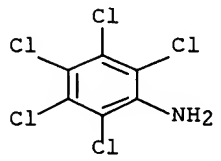
RN 95-76-1 HCAPLUS
CN Benzenamine, 3,4-dichloro- (9CI) (CA INDEX NAME)



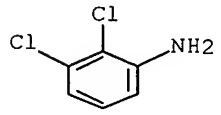
RN 108-70-3 HCAPLUS
CN Benzene, 1,3,5-trichloro- (8CI, 9CI) (CA INDEX NAME)



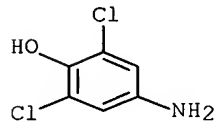
RN 527-20-8 HCAPLUS
CN Benzenamine, 2,3,4,5,6-pentachloro- (9CI) (CA INDEX NAME)



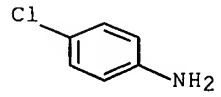
RN 608-27-5 HCAPLUS
CN Benzenamine, 2,3-dichloro- (9CI) (CA INDEX NAME)



RN 5930-28-9 HCAPLUS
CN Phenol, 4-amino-2,6-dichloro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IT **106-47-8P**, 4-Chloroaniline, biological studies
(residues of, leaching of, from soil)
RN 106-47-8 HCAPLUS
CN Benzenamine, 4-chloro- (9CI) (CA INDEX NAME)



CC 5-6 (Agrochemical Bioregulators)
Section cross-reference(s): 19
IT 87-40-1P, 2,4,6-Trichloroanisole 88-06-2P, 2,4,6-Trichlorophenol
95-57-8P, 2-Chlorophenol **95-76-1P**, 3,4-Dichloroaniline
100-66-3DP, Anisole, dichloro derivative 106-48-9P, 4-Chlorophenol
108-43-0P, 3-Chlorophenol **108-70-3P**,

1,3,5-Trichlorobenzene 120-14-9P, 3,4-Dimethoxybenzaldehyde 121-33-5P, Vanillin **527-20-8P**, Pentachloroaniline 539-03-7P 555-16-8P, 4-Nitrobenzaldehyde, biological studies **608-27-5P**, 2,3-Dichloroaniline 634-90-2P 933-78-8P, 2,3,5-Trichlorophenol 2621-62-7P **5930-28-9P**, 2,6-Dichloro-4-aminophenol 6130-75-2P, 2,4,5-Trichloroanisole 6851-44-1P 6975-29-7P, 2,4-Dichloroacetanilide 29191-52-4DP, Anisidine, chloro derivs. 50375-10-5P, 2,3,6-Trichloroanisole 54135-81-8P, 2,3,5-Trichloroanisole 54135-82-9P, 3,4,5-Trichloroanisole
(pentachloronitrobenzene degradation product, leaching of, from soil)

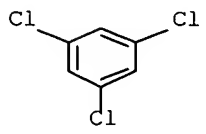
IT **106-47-8P**, 4-Chloroaniline, biological studies 82-68-8P, Pentachloronitrobenzene 309-00-2P, Aldrin 3766-60-7P, Buturon
(residues of, leaching of, from soil)

L64 ANSWER 33 OF 55 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1987:84102 HCAPLUS Full-text
DOCUMENT NUMBER: 106:84102
TITLE: Cobalt carbonyl-catalyzed polycarbonylation of aryl halides in sodium methoxide/methanol under photostimulation
AUTHOR(S): Kashimura, Tsugunori; Kudo, Kiyoshi; Mori, Sadayuki; Sugita, Nobuyuki
CORPORATE SOURCE: Inst. Chem. Res., Kyoto Univ., Uji, 611, Japan
SOURCE: Chemistry Letters (**1986**), (6), 851-4
CODEN: CMLTAG; ISSN: 0366-7022
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 106:84102

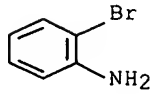
AB Cobalt carbonyl-catalyzed carbonylation of mono- and polychloro- and bromobenzenes and their derivs. occurred in NaOMe/MeOH under photostimulation to give Me esters of polycarboxylic acids. E.g., 3,4-Cl2C6H3CO2Me was irradiated in NaOMe/MeOH in the presence of Co2(CO)8 to give 1,2,4-(MeO2C)3C6H3. Carbonylation at the ortho position (to another halogen atom or carboxyl group) proceeds in high selectivity.

IT **108-70-3**, 1,3,5-Trichlorobenzene **615-36-1**, 2-Bromoaniline
(photocarbonylation of, Me esters from)

RN 108-70-3 HCAPLUS
CN Benzene, 1,3,5-trichloro- (8CI, 9CI) (CA INDEX NAME)



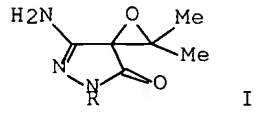
RN 615-36-1 HCAPLUS
CN Benzenamine, 2-bromo- (9CI) (CA INDEX NAME)



CC 25-18 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

IT 87-61-6, 1,2,3-Trichlorobenzene 95-46-5, 2-Bromotoluene 95-49-8, 2-Chlorotoluene 95-50-1, 1,2-Dichlorobenzene 95-94-3, 1,2,4,5-Tetrachlorobenzene 106-46-7 **108-70-3**, 1,3,5-Trichlorobenzene 120-82-1, 1,2,4-Trichlorobenzene 541-73-1, 1,3-Dichlorobenzene 578-57-4, 2-Bromoanisole 583-53-9, 1,2-Dibromobenzene 610-94-6, Methyl 2-bromobenzoate 610-96-8, Methyl 2-chlorobenzoate **615-36-1**, 2-Bromoaniline 694-80-4, 2-Chlorobromobenzene 766-51-8, 2-Chloroanisole 2905-68-2, Methyl 3,4-dichlorobenzoate 35112-28-8, Methyl 2,4-dichlorobenzoate 106727-86-0
(photocarbonylation of, Me esters from)

L64 ANSWER 34 OF 55 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1986:590558 HCAPLUS Full-text
DOCUMENT NUMBER: 105:190558
TITLE: New azoolefins and their acidic cleavage to aryldiimines
AUTHOR(S): Kirschke, Klaus; Moeller, Angela; Schmitz, Ernst
CORPORATE SOURCE: Zentralinst. Org. Chem., Dtsch. Akad. Wiss., Berlin-Adlershof, DDR-1199, Ger. Dem. Rep.
SOURCE: Journal fuer Praktische Chemie (Leipzig) (**1985**), 327(6), 893-92
CODEN: JPCEAO; ISSN: 0021-8383
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 105:190558
GI



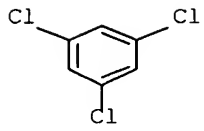
I

AB Pyrazolinespirooxiranones I (R = Ph, 2,5-Cl2C6H3, 2,4,6-Cl3C6H2) underwent ring opening with NaOMe to give RN:NC(NH2):CHCO2Me (II). II were cleaved under amidic conditions. The main products of the cleavage of II (R = 2,4,6-Cl3C6H2) with MeOH-HCl are N, 1,3,5-Cl3C6H3, 2,4,6-Cl3C6H2NH2 and 2,4,6-Cl3C6H2NHNH2. Intermediates of the cleavage of II were aryldiimines which were trapped with PhCHO to give BzNHNHR (R = 2,5-Cl2C6H3, 2,4,6-Cl3C6H2).

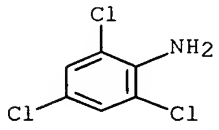
IT **108-70-3P 634-93-5P**
(formation of, in cleavage of amino(trichlorophenylazo)propenoate)

RN 108-70-3 HCAPLUS

CN Benzene, 1,3,5-trichloro- (8CI, 9CI) (CA INDEX NAME)



RN 634-93-5 HCAPLUS
CN Benzenamine, 2,4,6-trichloro- (9CI) (CA INDEX NAME)



CC 25-5 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 28
IT **108-70-3P 634-93-5P** 2724-66-5P 5329-12-4P
18490-44-3P
(formation of, in cleavage of amino(trichlorophenylazo)propenoate)

L64 ANSWER 35 OF 55 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1984:406801 HCAPLUS Full-text
DOCUMENT NUMBER: 101:6801
TITLE: Halo-anilines
INVENTOR(S): Ratton, Serge
PATENT ASSIGNEE(S): Rhone-Poulenc Agrochimie, Fr.
SOURCE: Fr. Demande, 11 pp.
CODEN: FRXXBL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2529198	A1	19831230	FR 1982-11617	19820629
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FR 2529198	B1	19850329		
IL 68943	A1	19860731	IL 1983-68943	19830609
			<--	
EP 98783	A1	19840118	EP 1983-420103	19830621
			<--	
EP 98783	B1	19850821		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
AT 15030	E	19850915	AT 1983-420103	

				1983
				0621
			<--	
ZA 8304690	A	19840328	ZA 1983-4690	
				1983
				0627
			<--	
CA 1209589	A1	19860812	CA 1983-431209	
				1983
				0627
			<--	
DK 8302971	A	19831230	DK 1983-2971	
				1983
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DK 161069	B	19910527		
DK 161069	C	19911118		
JP 59013750	A2	19840124	JP 1983-116831	
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				0628
			<--	
JP 02058253	B4	19901207		
BR 8303461	A	19840207	BR 1983-3461	
				1983
				0628
			<--	
DD 210030	A5	19840530	DD 1983-252467	
				1983
				0628
			<--	
ES 523638	A1	19840816	ES 1983-523638	
				1983
				0628
			<--	
US 4508922	A	19850402	US 1983-508716	
				1983
				0628
			<--	
HU 32330	O	19840730	HU 1983-2363	
				1983
				0629
			<--	
HU 190495	B	19860929		
PRIORITY APPLN. INFO.:			FR 1982-11617	A
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				0629
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			EP 1983-420103	A
				1983
				0621
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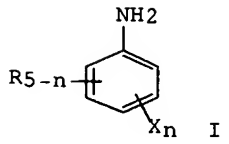
OTHER SOURCE(S):	MARPAT 101:6801			
GI				



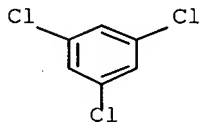
I

AB Halobenzenes were treated with NH3 and catalysts obtained from Cu and 8-hydroxyquinolines to yield anilines I (n = 0, 1, 2, 3, 4, 5; X = same or different halo; R = H, alkyl, alkoxy). Thus, 1,3,5-Cl3C6H3 was treated with NH3, CuCl, and 8-hydroxyquinoline to give 3,5-Cl2C6H3NH2.

IT **108-70-3**
(ammonolysis of, catalysts for)

RN 108-70-3 HCAPLUS

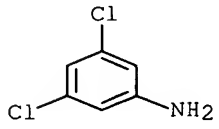
CN Benzene, 1,3,5-trichloro- (8CI, 9CI) (CA INDEX NAME)



IT **626-43-7P**
(preparation of)

RN 626-43-7 HCAPLUS

CN Benzenamine, 3,5-dichloro- (9CI) (CA INDEX NAME)



IC C07C087-60; C07C085-04

CC 25-4 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

IT **108-70-3** 108-90-7, reactions
(ammonolysis of, catalysts for)

IT **626-43-7P**
(preparation of)

L64 ANSWER 36 OF 55 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1984:209256 HCAPLUS Full-text

DOCUMENT NUMBER: 100:209256

TITLE: High-resolution PCB analysis: synthesis and chromatographic properties of all 209 PCB congeners

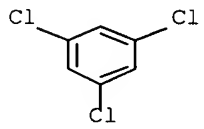
AUTHOR(S): Mullins, Michael D.; Pochini, Cynthia M.; McCrindle, Shelia; Romkes, Marjorie; Safe, Stephen H.; Safe, Lorna M.

CORPORATE SOURCE: Large Lakes Res. Stn., U. S. Environ. Prot.

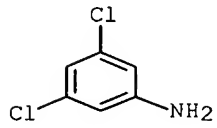
Agency, Grosse Ile, MI, 48138, USA
SOURCE: Environmental Science and Technology (**1984**), 18(6), 468-76
CODEN: ESTHAG; ISSN: 0013-936X
DOCUMENT TYPE: Journal
LANGUAGE: English

AB This paper reports the synthesis and spectroscopic properties of all the mono-, di-, tri-, tetra-, penta-, hexa-, and heptachlorobiphenyls and completes the synthesis of all 209 polychlorinated biphenyls (PCBs). The retention times and molar response factors of the 209 PCGs were determined relative to a reference standard, octachloronaphthalene. The retention times for these compds. generally increased with increasing Cl content, and it was apparent that within a series of isomers there was an increase in retention time with increasing meta and para and decreasing ortho substitution. By use of a 50-m narrow bore fused silica capillary column coated with SE-54, it was possible to sep. 187 PCB congeners, and only 11 pairs of compds. were not fully resolved. With some addnl. anal. improvements, isomer-specific PCB anal. can be utilized to determine the composition of com. PCBs and accurately follow the fate and distribution of these pollutants within the global ecosystem.

IT **108-70-3**
(coupling of, with diazotized aniline or chloroanilines)
RN 108-70-3 HCAPLUS
CN Benzene, 1,3,5-trichloro- (8CI, 9CI) (CA INDEX NAME)



IT **626-43-7**
(diazotization-coupling of, with benzene or chlorobenzenes)
RN 626-43-7 HCAPLUS
CN Benzenamine, 3,5-dichloro- (9CI) (CA INDEX NAME)



CC 25-3 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 19, 59, 60, 80
IT 71-43-2, reactions 87-61-6 95-50-1 95-94-3 106-46-7
108-70-3 108-90-7, reactions 120-82-1 541-73-1
608-93-5 634-66-2 634-90-2
(coupling of, with diazotized aniline or chloroanilines)
IT 62-53-3, reactions 95-51-2 95-76-1 95-82-9 106-47-8,
reactions 108-42-9 527-20-8 554-00-7 608-27-5 608-31-1
626-43-7 634-67-3 634-83-3 634-91-3 634-93-5
636-30-6 654-36-4 3481-20-7 88963-39-7
(diazotization-coupling of, with benzene or chlorobenzenes)

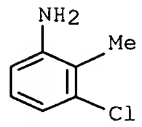
L64 ANSWER 37 OF 55 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1984:191552 HCAPLUS Full-text
DOCUMENT NUMBER: 100:191552
TITLE: Aromatic chlorine derivatives
INVENTOR(S): Lerke, Andrzej; Pilecka, Danuta; Kopka, Ewa; Raatz, Bernard; Stasiak, Jan; Kubiak, Alfons
PATENT ASSIGNEE(S): Zaklady Chemiczne "Organika-Zachem", Pol.
SOURCE: Pol., 4 pp.
CODEN: POXXA7
DOCUMENT TYPE: Patent
LANGUAGE: Polish
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PL 120348	B1	19820227	PL 1978-211630	1978 1211 <--

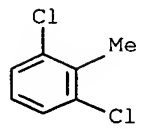
PRIORITY APPLN. INFO.: PL 1978-211630 1978 1211 <--

AB Chlorobenzenes were prepared from anilines by Sandmeyer diazotization in the presence of 4-9:1 NaCl-CuCl. The process was illustrated in terms of a numbered diagram. Data were given for conversion of 4,3-Me(O2N)C6H3NH2, 2,5-Me(O2N)C6H3NH2, 3,2-ClMeC6H3NH2, 5,2-ClMeC6H3NH2, and 2-MeC6H4NH2 into the corresponding chlorobenzenes.

IT **87-60-5**
(Sandmeyer reaction of)
RN 87-60-5 HCAPLUS
CN Benzenamine, 3-chloro-2-methyl- (9CI) (CA INDEX NAME)



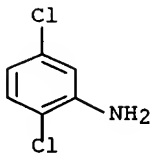
IT **118-69-4P**
(preparation of)
RN 118-69-4 HCAPLUS
CN Benzene, 1,3-dichloro-2-methyl- (9CI) (CA INDEX NAME)



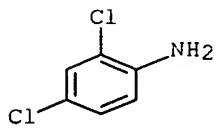
IC C07C025-02; C07C079-12

CC 25-3 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
IT **87-60-5** 95-53-4, reactions 95-79-4 99-55-8
119-32-4
(Sandmeyer reaction of)
IT 89-59-8P 95-49-8P 95-73-8P **118-69-4P** 121-86-8P
(preparation of)

L64 ANSWER 38 OF 55 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1984:50832 HCAPLUS Full-text
DOCUMENT NUMBER: 100:50832
TITLE: Synthesis and characterization of twenty-two purified polychlorinated dibenzofuran congeners
AUTHOR(S): Safe, Stephen H.; Safe, Lorna M.
CORPORATE SOURCE: Coll. Vet. Med., Texas A and M Univ., College Station, TX, 77843, USA
SOURCE: Journal of Agricultural and Food Chemistry (**1984**), 32(1), 68-71
CODEN: JAFCAU; ISSN: 0021-8561
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 100:50832
AB Polychlorinated dibenzofurans (PCDF) were prepared by the base-catalyzed cyclization of the corresponding hydroxypolychlorinated biphenyl (PCB) precursors containing ortho chloro and hydroxy substituents on the 2 Ph rings. The hydroxy PCBs were prepared from the methoxy analogs by the diazo coupling of either chlorinated anisidines and sym. chlorinated benzenes or of chlorinated anilines and chlorinated anisoles.
IT **95-82-9 554-00-7 608-27-5**
608-31-1 634-67-3 634-83-3
636-30-6 3481-20-7
(coupling of, with anisole, and demethylation and ring closure of)
RN 95-82-9 HCAPLUS
CN Benzenamine, 2,5-dichloro- (9CI) (CA INDEX NAME)

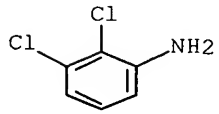


RN 554-00-7 HCAPLUS
CN Benzenamine, 2,4-dichloro- (9CI) (CA INDEX NAME)

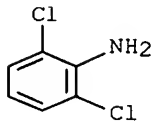


RN 608-27-5 HCAPLUS

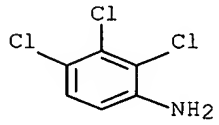
CN Benzenamine, 2,3-dichloro- (9CI) (CA INDEX NAME)



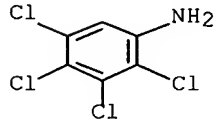
RN 608-31-1 HCAPLUS
CN Benzenamine, 2,6-dichloro- (9CI) (CA INDEX NAME)



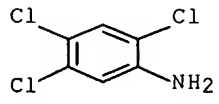
RN 634-67-3 HCAPLUS
CN Benzenamine, 2,3,4-trichloro- (9CI) (CA INDEX NAME)



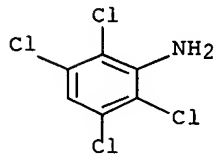
RN 634-83-3 HCAPLUS
CN Benzenamine, 2,3,4,5-tetrachloro- (9CI) (CA INDEX NAME)



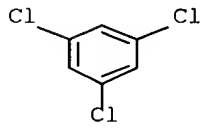
RN 636-30-6 HCAPLUS
CN Benzenamine, 2,4,5-trichloro- (9CI) (CA INDEX NAME)



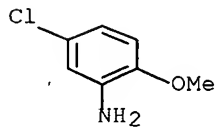
RN 3481-20-7 HCAPLUS
CN Benzenamine, 2,3,5,6-tetrachloro- (9CI) (CA INDEX NAME)



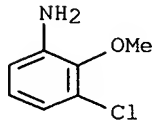
IT **108-70-3**
(coupling of, with chlorinated anisidine, and demethylation and ring closure of)
RN 108-70-3 HCAPLUS
CN Benzene, 1,3,5-trichloro- (8CI, 9CI) (CA INDEX NAME)



IT **95-03-4 51114-68-2**
(coupling of, with chlorinated benzene, and demethylation and cyclization of)
RN 95-03-4 HCAPLUS
CN Benzenamine, 5-chloro-2-methoxy- (9CI) (CA INDEX NAME)



RN 51114-68-2 HCAPLUS
CN Benzenamine, 3-chloro-2-methoxy- (9CI) (CA INDEX NAME)



CC 22-6 (Physical Organic Chemistry)
IT **95-82-9 554-00-7 608-27-5**
608-31-1 634-67-3 634-83-3
636-30-6 2683-43-4 **3481-20-7**

(coupling of, with anisole, and demethylation and ring closure of)

IT 95-94-3 106-46-7 **108-70-3** 608-93-5 634-66-2
(coupling of, with chlorinated anisidine, and demethylation and ring closure of)

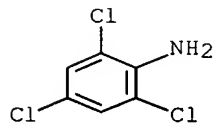
IT **95-03-4 51114-68-2**
(coupling of, with chlorinated benzene, and demethylation and cyclization of)

L64 ANSWER 39 OF 55 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1982:51945 HCAPLUS Full-text
DOCUMENT NUMBER: 96:51945
TITLE: Reduction of aryldiazonium salts to arenes
AUTHOR(S): Lahoti, R. J.; Parameswaran, V.; Wagle, D. R.
CORPORATE SOURCE: Natl. Chem. Lab., Poona City, 411 008, India
SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (**1981**), 20B(9), 767-9
CODEN: IJSBDB; ISSN: 0376-4699
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 96:51945

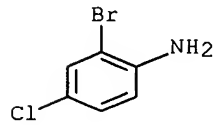
AB Aryldiazonium fluoroborates were smoothly reduced to the corresponding hydrocarbon derivs. by warming with DMF. When the amine has an electron donating substituent, the reaction proceeds at 65°. When the amine has electron withdrawing substituents, the reaction proceeds rapidly at 25-45°. Deamination of 2,4,6-trichlorobenzenediazonium fluoroborate with tetramethylurea gave AcH, an unexpected product, and 3,5-Cl2C6H3Cl. The amines were also deaminated with DMF without separation of the diazonium salt in aqueous or non-aqueous medium.

IT **634-93-5 873-38-1**
(diazotization of)

RN 634-93-5 HCAPLUS
CN Benzenamine, 2,4,6-trichloro- (9CI) (CA INDEX NAME)



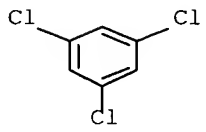
RN 873-38-1 HCAPLUS
CN Benzenamine, 2-bromo-4-chloro- (9CI) (CA INDEX NAME)



IT **108-70-3P**
(preparation of, by reduction of diazonium salt with DMF)

RN 108-70-3 HCAPLUS

CN Benzene, 1,3,5-trichloro- (8CI, 9CI) (CA INDEX NAME)



CC 25-27 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 26

IT 60-09-3 88-05-1 91-59-8 97-02-9 99-30-9 100-01-6, reactions 102-56-7 145-49-3 610-41-3 **634-93-5** 719-59-5 **873-38-1** 3224-33-7 6925-48-0 80468-91-3
(diazotization of)

IT 98-95-3P, preparation 99-65-0P 103-33-3P 108-37-2P 108-67-8P, preparation **108-70-3P** 117-12-4P 150-78-7P 528-29-0P 1016-78-0P 1562-93-2P 80468-92-4P 80468-93-5P
(preparation of, by reduction of diazonium salt with DMF)

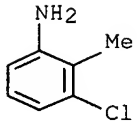
L64 ANSWER 40 OF 55 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1982:6344 HCAPLUS Full-text
DOCUMENT NUMBER: 96:6344
TITLE: Aryl chlorides
INVENTOR(S): Lanet, Jean Claude; Bourdon, Jacques
PATENT ASSIGNEE(S): Rhone-Poulenc Industries S. A., Fr.
SOURCE: Fr. Demande, 12 pp.
CODEN: FRXXBL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2475535	A1	19810814	FR 1980-2652	19800207
			<--	
FR 2475535	B1	19830805		
PRIORITY APPLN. INFO.:			FR 1980-2652 A	19800207
			<--	

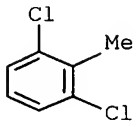
AB Aryl chlorides were prepared from corresponding anilines by Sandmeyer halogenation in the presence of metallic Fe and/or and Fe(II) salt. The CuCl-Fe(II) mol ratio was 0.1-5. The surface area of the metallic Fe was >15 cm3/L of solution Thus, 2,6-Cl(H2N)C6H3Me was converted to the diazonium salt, which was decomposed in the presence CuCl-Fe or CuCl-FeCl2 to give 2,6-Cl2C6H3Me in 80.2 and 73.6% yield, resp.

IT **87-60-5**
(diazotization of)

RN 87-60-5 HCAPLUS
CN Benzenamine, 3-chloro-2-methyl- (9CI) (CA INDEX NAME)

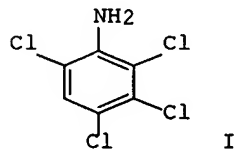


IT **118-69-4P**
(preparation of)
RN 118-69-4 HCAPLUS
CN Benzene, 1,3-dichloro-2-methyl- (9CI) (CA INDEX NAME)



IC C07C025-02; C07C017-22
CC 25-3 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
IT 62-53-3, reactions **87-60-5** 90-04-0 106-49-0, reactions
(diazotization of)
IT **118-69-4P** 766-51-8P
(preparation of)

L64 ANSWER 41 OF 55 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1981:474712 HCAPLUS Full-text
DOCUMENT NUMBER: 95:74712
TITLE: Synthesis of the octa- and nonachlorobiphenyl isomers and congeners and their quantitation in commercial polychlorinated biphenyls and identification in human breast milk
AUTHOR(S): Mullin, M.; Sawka, G.; Safe, L.; McCrindle, S.; Safe, S.
CORPORATE SOURCE: Large Lakes Res. Stn., EPA, Grosse Ile, MI, 48138, USA
SOURCE: Journal of Analytical Toxicology (**1981**), 5(3), 138-42
CODEN: JATOD3; ISSN: 0146-4760
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



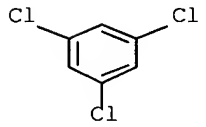
I

AB The synthesis of all possible isomeric nona- and octachlorobiphenyls was accomplished by the Cadogan coupling of com. available or synthetic chlorinated anilines in the presence of excess chlorinated benzenes and isoamyl nitrite. 2,3,4,6-Tetrachloroaniline (I) [**654-36-4**] was prepared by the chlorination of 2,4,5-trichloroaniline [**636-30-6**]. The synthetic PCBs were characterized by their proton magnetic resonance and mass spectra and their purities determined by gas chromatog. analyses. The PCB stds. were used to unambiguously identify the deca-, nona-, and octachlorobiphenyls present in human breast milk and in the com. PCB prepns. Aroclor 1268 [11100-14-4], 1262 [37324-23-5], 1260 [11096-82-5], 1254 [11097-69-1], 1248 [12672-29-6], 1242 [53469-21-9], 1016 [12674-11-2], 1232 [11141-16-5] and 1221 [11104-28-2] utilizing high resolution glass capillary gas chromatog.

IT **108-70-3**
(reaction of, with chloroanilines)

RN 108-70-3 HCAPLUS

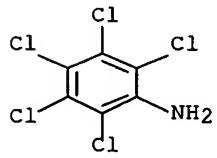
CN Benzene, 1,3,5-trichloro- (8CI, 9CI) (CA INDEX NAME)



IT **527-20-8 634-67-3 634-83-3**
634-91-3 636-30-6 654-36-4
3481-20-7
(reaction of, with chlorobenzenes)

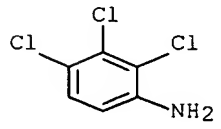
RN 527-20-8 HCAPLUS

CN Benzenamine, 2,3,4,5,6-pentachloro- (9CI) (CA INDEX NAME)



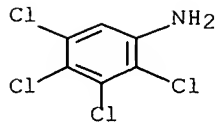
RN 634-67-3 HCAPLUS

CN Benzenamine, 2,3,4-trichloro- (9CI) (CA INDEX NAME)

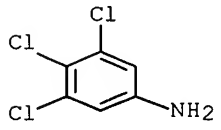


RN 634-83-3 HCAPLUS

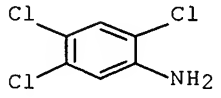
CN Benzenamine, 2,3,4,5-tetrachloro- (9CI) (CA INDEX NAME)



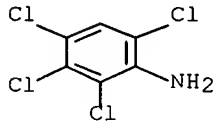
RN 634-91-3 HCAPLUS
CN Benzenamine, 3,4,5-trichloro- (9CI) (CA INDEX NAME)



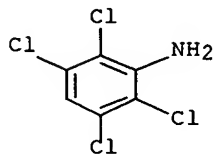
RN 636-30-6 HCAPLUS
CN Benzenamine, 2,4,5-trichloro- (9CI) (CA INDEX NAME)



RN 654-36-4 HCAPLUS
CN Benzenamine, 2,3,4,6-tetrachloro- (9CI) (CA INDEX NAME)



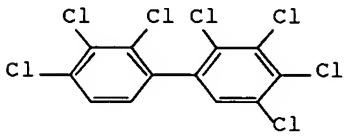
RN 3481-20-7 HCAPLUS
CN Benzenamine, 2,3,5,6-tetrachloro- (9CI) (CA INDEX NAME)



CC 4-1 (Toxicology)
Section cross-reference(s): 25

IT 95-94-3 **108-70-3** 120-82-1 608-93-5 634-66-2
634-90-2
(reaction of, with chloroanilines)
IT **527-20-8 634-67-3 634-83-3**
634-91-3 636-30-6 654-36-4
3481-20-7
(reaction of, with chlorobenzenes)

L64 ANSWER 42 OF 55 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1981:419101 HCAPLUS Full-text
DOCUMENT NUMBER: 95:19101
TITLE: Polychlorinated biphenyls as inducers of hepatic microsomal enzymes: effects of di-ortho substitution
AUTHOR(S): Parkinson, A.; Robertson, L. W.; Safe, Lorna; Safe, S.
CORPORATE SOURCE: Guelph-Waterloo Cent. Grad. Work Chem., Univ. Guelph, Guelph, ON, N1G 2W1, Can.
SOURCE: Chemico-Biological Interactions (**1981**), 35(1), 1-12
CODEN: CBINA8; ISSN: 0009-2797
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



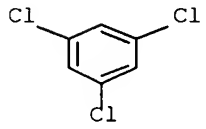
I

AB All of the 13 possible PCB isomers and congeners substituted at both para positions, at least 2 meta positions (but not necessarily on the same ring), and at 2 ortho positions were synthesized and tested as rat hepatic microsomal enzyme inducers. The effects of the compds. were evaluated by measuring microsomal benzo[a]pyrene hydroxylase (B[a]P hydroxylase) [9037-52-9], 4-chlorobiphenyl hydroxylase (4-CBP hydroxylase) [77967-77-2], 4-dimethylaminoantipyrine N-demethylase (DMAP N-demethylase) [73299-01-1], and NADPH-cytochrome c reductase [9023-03-4] activities, the cytochrome b5 [9035-39-6] content and the relative peak intensities and spectral shifts of the CO and ethylisocyanide(EIC)-difference spectra of ferrocytochrome P 450. The results were compared to the effects of administering phenobarbitone (PB), 3-methylcholanthrene (MC) and PB + MC. At dose levels of 150 μmol/kg, all of the PCB congeners, except 2,3',4,4',5',6-hexachlorobiphenyl [59291-65-5], significantly enhanced hepatic microsomal cytochrome P 450 [9035-51-2] content, B[a]P hydroxylase and/or DMAP N-demethylase activities compared to the control (corn oil-treated) animals. Only 5 of these compds., namely 2,3,4,4',5,6-hexa- [41411-63-6], 2,2',3,3',4,4'-hexa- [38380-07-3], 2,2',3',4,4',5-hexa- [35694-06-5], 2,3,3',4,4',6-hexa [74472-42-7], and 2,2',3,3',4,4',5- heptachlorobiphenyl (I) [52663-74-8], enhanced microsomal B[a]P hydroxylase, 4-CBP hydroxylase, NADPH-cytochrome c reductase, and DMAP N-demethylase activities in a manner consistent with a mixed pattern of induction. Thus, PCB isomers and congeners substituted at both para positions, at least 2 meta positions, at 2 ortho positions and containing a

2,3,4-trichloro substitution pattern on 1 ring are mixed-type inducers; in addition the effects of 2,3,4,4',5,6-hexachlorobiphenyl were also consistent with a mixed pattern of induction.

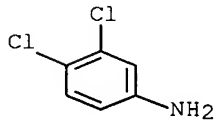
IT **108-70-3**
(reaction of, with haloanilines)

RN 108-70-3 HCAPLUS
CN Benzene, 1,3,5-trichloro- (8CI, 9CI) (CA INDEX NAME)

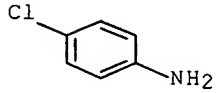


IT **95-76-1 106-47-8**, biological studies
554-00-7 634-67-3 634-83-3
634-91-3 636-30-6
(reaction of, with halobenzenes)

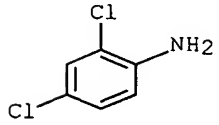
RN 95-76-1 HCAPLUS
CN Benzenamine, 3,4-dichloro- (9CI) (CA INDEX NAME)



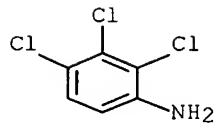
RN 106-47-8 HCAPLUS
CN Benzenamine, 4-chloro- (9CI) (CA INDEX NAME)



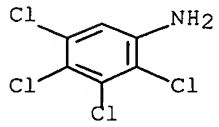
RN 554-00-7 HCAPLUS
CN Benzenamine, 2,4-dichloro- (9CI) (CA INDEX NAME)



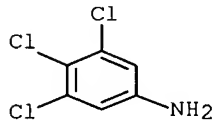
RN 634-67-3 HCAPLUS
CN Benzenamine, 2,3,4-trichloro- (9CI) (CA INDEX NAME)



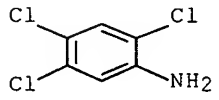
RN 634-83-3 HCAPLUS
CN Benzenamine, 2,3,4,5-tetrachloro- (9CI) (CA INDEX NAME)



RN 634-91-3 HCAPLUS
CN Benzenamine, 3,4,5-trichloro- (9CI) (CA INDEX NAME)



RN 636-30-6 HCAPLUS
CN Benzenamine, 2,4,5-trichloro- (9CI) (CA INDEX NAME)

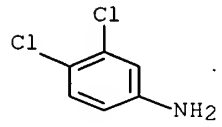


CC 4-3 (Toxicology)
Section cross-reference(s): 25
IT 87-61-6 **108-70-3** 608-93-5 634-66-2 634-90-2
(reaction of, with haloanilines)
IT **95-76-1 106-47-8**, biological studies
554-00-7 634-67-3 634-83-3
634-91-3 636-30-6 62720-28-9
(reaction of, with halobenzenes)

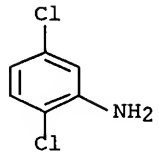
L64 ANSWER 43 OF 55 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1981:139338 HCAPLUS Full-text
DOCUMENT NUMBER: 94:139338
TITLE: Synthesis of monosubstituted chlorobenzenes by photoinduced dechlorination
AUTHOR(S): Mansour, Mohammed; Wawrik, Silvia; Parlar,

Harun; Korte, Friedhelm
CORPORATE SOURCE: Inst. Oekol. Chem., Ges. Strahlen- und Umweltforsch. m.b.H. Muenchen, Freising-Attaching, Fed. Rep. Ger.
SOURCE: Chemiker-Zeitung (**1980**), 104(11), 339-40
CODEN: CMKZAT; ISSN: 0009-2894
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 94:139338
AB Irradiating dichlorobenzenes Cl2C6H3R (R = H, Me, CH2OH, MeO, OH, NH2, Ph) (22 compds.), in MeOH above 230 nm resulted in monodechlorination to give ClC6H4R in 5-67% yield.
IT **95-76-1 95-82-9 118-69-4 554-00-7**
(photolytic monodechlorination of)

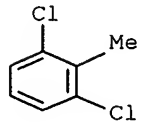
RN 95-76-1 HCAPLUS
CN Benzenamine, 3,4-dichloro- (9CI) (CA INDEX NAME)



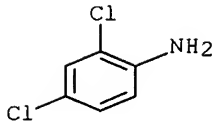
RN 95-82-9 HCAPLUS
CN Benzenamine, 2,5-dichloro- (9CI) (CA INDEX NAME)



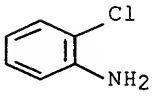
RN 118-69-4 HCAPLUS
CN Benzene, 1,3-dichloro-2-methyl- (9CI) (CA INDEX NAME)



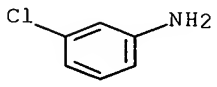
RN 554-00-7 HCAPLUS
CN Benzenamine, 2,4-dichloro- (9CI) (CA INDEX NAME)



IT **95-51-2P 108-42-9P**
(preparation of, by photodechlorination of dichloroaniline)
RN 95-51-2 HCAPLUS
CN Benzenamine, 2-chloro- (9CI) (CA INDEX NAME)



RN 108-42-9 HCAPLUS
CN Benzenamine, 3-chloro- (9CI) (CA INDEX NAME)

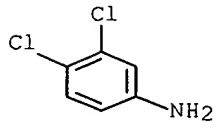


CC 25-2 (Noncondensed Aromatic Compounds)
IT 87-65-0 95-50-1 95-73-8 **95-76-1** 95-77-2
95-82-9 106-46-7 **118-69-4** 541-73-1
554-00-7 583-78-8 591-35-5 1777-82-8 1805-32-9
1984-59-4 1984-65-2 16605-91-7 19398-61-9 33284-50-3
33719-74-3 34883-41-5
(photolytic monodechlorination of)
IT **95-51-2P 108-42-9P**
(preparation of, by photodechlorination of dichloroaniline)

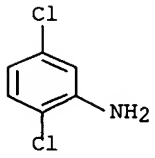
L64 ANSWER 44 OF 55 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1980:471153 HCAPLUS Full-text
DOCUMENT NUMBER: 93:71153
TITLE: Photoinduced deuteration of monosubstituted dichlorobenzenes
AUTHOR(S): Mansour, Mohammed; Parlar, Harun; Korte, Friedhelm
CORPORATE SOURCE: Inst. Oekol. Chem., Ges. Strahlen- und Umweltforsch. m.b.H. Muenchen, Freising-Attaching, D-8050, Fed. Rep. Ger.
SOURCE: Chemosphere (**1980**), 9(1), 59-60
CODEN: CMSHAF; ISSN: 0045-6535
DOCUMENT TYPE: Journal
LANGUAGE: German
AB Dichlorobenzene isomers and their monosubstituted derivs. (30 compds.) underwent exchange of one of the Cl atoms with D by photolyzing in CD3OD for 10-240 min. Product yields were <67%.

IT **95-76-1 95-82-9 118-69-4**
554-00-7 608-27-5 608-31-1
(deuteration of, monodechlorination in)

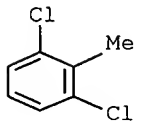
RN 95-76-1 HCAPLUS
CN Benzenamine, 3,4-dichloro- (9CI) (CA INDEX NAME)



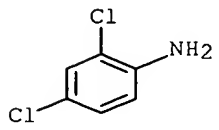
RN 95-82-9 HCAPLUS
CN Benzenamine, 2,5-dichloro- (9CI) (CA INDEX NAME)



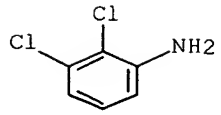
RN 118-69-4 HCAPLUS
CN Benzene, 1,3-dichloro-2-methyl- (9CI) (CA INDEX NAME)



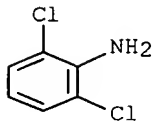
RN 554-00-7 HCAPLUS
CN Benzenamine, 2,4-dichloro- (9CI) (CA INDEX NAME)



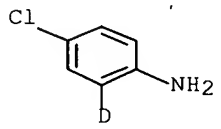
RN 608-27-5 HCAPLUS
CN Benzenamine, 2,3-dichloro- (9CI) (CA INDEX NAME)



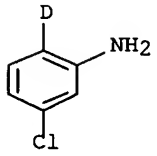
RN 608-31-1 HCAPLUS
CN Benzenamine, 2,6-dichloro- (9CI) (CA INDEX NAME)



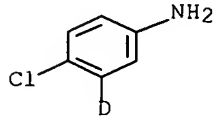
IT **74383-34-9P 74383-35-0P 74383-36-1P**
74383-37-2P 74383-38-3P
(preparation of)
RN 74383-34-9 HCAPLUS
CN Benzen-2-d-amine, 4-chloro- (9CI) (CA INDEX NAME)



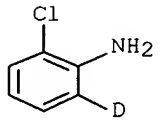
RN 74383-35-0 HCAPLUS
CN Benzen-2-d-amine, 5-chloro- (9CI) (CA INDEX NAME)



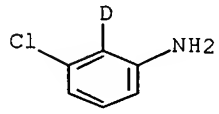
RN 74383-36-1 HCAPLUS
CN Benzen-3-d-amine, 4-chloro- (9CI) (CA INDEX NAME)



RN 74383-37-2 HCAPLUS
CN Benzen-2-d-amine, 6-chloro- (9CI) (CA INDEX NAME)



RN 74383-38-3 HCAPLUS
CN Benzen-2-d-amine, 3-chloro- (9CI) (CA INDEX NAME)



CC 25-3 (Noncondensed Aromatic Compounds)
IT 87-65-0 95-50-1 **95-76-1** 95-77-2 **95-82-9**
106-46-7 **118-69-4** 541-73-1 **554-00-7**
583-78-8 591-35-5 **608-27-5** **608-31-1**
611-06-3 874-42-0 1194-65-6 1777-82-8 1805-32-9
1984-59-4 1984-65-2 3209-22-1 6287-38-3 16605-91-7
19398-61-9 25186-47-4 32768-54-0 33284-50-3 33719-74-3
34883-39-1 34883-41-5
(deuteration of, monodechlorination in)
IT 2401-28-7P 13122-34-4P 15733-68-3P 19256-46-3P 19256-47-4P
74383-21-4P 74383-22-5P 74383-23-6P 74383-24-7P
74383-25-8P 74383-26-9P 74383-27-0P 74383-28-1P
74383-29-2P 74383-30-5P 74383-31-6P 74383-32-7P
74383-33-8P **74383-34-9P** **74383-35-0P**
74383-36-1P **74383-37-2P** **74383-38-3P**
74383-39-4P 74383-40-7P 74383-41-8P 74383-42-9P
74383-43-0P 74398-87-1P 74398-88-2P
(preparation of)

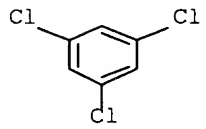
L64 ANSWER 45 OF 55 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1979:574945 HCAPLUS Full-text
DOCUMENT NUMBER: 91:174945
TITLE: Synthesis of 2,4-dimethoxy-5-chloroaniline
AUTHOR(S): Boc, I.; Palea, R.; Arion, D.; Todoran, M.
CORPORATE SOURCE: Inst. Politeh. "Traianvuia", Timisoara, Rom.
SOURCE: Lucr. Teh.-Stiint.: Chim. Tehnol. Chim., Ses. Comun. Festivalului "Cintarea Rom." (**1977**), 143-6. Inst. Politeh. "Traian Vuia": Timisoara, Rom.
CODEN: 41KIAX
DOCUMENT TYPE: Conference
LANGUAGE: Romanian

AB Nitration of a mixture of chlorobenzenes gave 2,4,5-Cl3C6H2NO2, which was methoxylated (MeOH-MeONa) and then reduced (Fe-aqueous FeCl2) to give 5,2,4-Cl(MeO)2C6H2NO2.

IT **108-70-3**
(nitration of)

RN 108-70-3 HCAPLUS

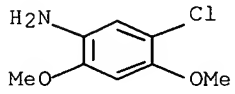
CN Benzene, 1,3,5-trichloro- (8CI, 9CI) (CA INDEX NAME)



IT **97-50-7P**
(preparation of)

RN 97-50-7 HCAPLUS

CN Benzenamine, 5-chloro-2,4-dimethoxy- (9CI) (CA INDEX NAME)



CC 25-10 (Noncondensed Aromatic Compounds)

IT 87-61-6 95-50-1 106-46-7 **108-70-3** 120-82-1
541-73-1 634-66-2 634-90-2
(nitration of)

IT **97-50-7P**
(preparation of)

L64 ANSWER 46 OF 55 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1979:71845 HCAPLUS Full-text

DOCUMENT NUMBER: 90:71845

TITLE: Partial amination of sym-trichlorobenzene with copper catalyst and trialkylamine

AUTHOR(S): Kamiyama, Tsutomu; Enomoto, Saburo; Inoue, Masami

CORPORATE SOURCE: Fac. Pharm. Sci., Toyama Med. Pharm. Univ., Toyama, Japan

SOURCE: Yuki Gosei Kagaku Kyokaishi (**1978**), 36(9), 784-8
CODEN: YGKKAE; ISSN: 0372-770X

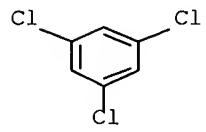
DOCUMENT TYPE: Journal

LANGUAGE: Japanese

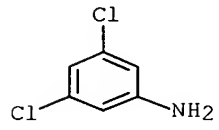
OTHER SOURCE(S): CASREACT 90:71845

AB In the Cu-catalyzed amination of sym-trichlorobenzene (I) with aqueous NH3 the presence of trialkylamines, e.g., Et3N, Pr3N, increased the yield of 3,5-dichloroaniline (II) relative to 3,5-diaminochlorobenzene (III). For example, heating a mixture of 5 g of I, 25 g of 28% NH4OH, 1 g of Cu, and 3 g of Et3N at 250° for 2 h converted 67.4% of I to II, III, and 1,3-dichlorobenzene in relative yields of 0.6, 86.9, and 12.5%, resp. Without Et3N, the relative yields were 2.9, 36.4, and 60.7% resp., and the conversion was 69.5%.

IT **108-70-3**
(amination of, catalytic)
RN 108-70-3 HCAPLUS
CN Benzene, 1,3,5-trichloro- (8CI, 9CI) (CA INDEX NAME)



IT **626-43-7P**
(preparation of, by amination of trichlorobenzene, catalytic)
RN 626-43-7 HCAPLUS
CN Benzenamine, 3,5-dichloro- (9CI) (CA INDEX NAME)



CC 25-4 (Noncondensed Aromatic Compounds)
IT 87-61-6 95-50-1 106-46-7 **108-70-3** 120-82-1
541-73-1
(amination of, catalytic)
IT **626-43-7P** 33786-89-9P
(preparation of, by amination of trichlorobenzene, catalytic)

L64 ANSWER 47 OF 55 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1979:54646 HCAPLUS Full-text
DOCUMENT NUMBER: 90:54646
TITLE: Chloroanilines
INVENTOR(S): Enomoto, Saburo; Inoue, Masami; Ueyama, Tsutomu
PATENT ASSIGNEE(S): Seitetsu Chemical Industry Co., Ltd., Japan; Sumitomo Chemical Co., Ltd.
SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 53121725	A2	19781024	JP 1977-37814	19770401
			<--	
JP 60048500	B4	19851028		

PRIORITY APPLN. INFO.: JP 1977-37814 A

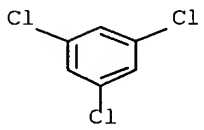
<--

AB Chloroanilines were prepared by partial substitution of polychlorobenzenes with NH3 in the presence of Cu-containing substances and tertiary amines. Thus, 1,3,5-Cl3C6H3 (I) 5, 28% aqueous NH3 29, Cu 1, and 30% aqueous Et3N 5 parts were autoclaved 2 h at 200° to give 29.0 mol% I, 41.9 mol% 3,5-Cl2C6H3NH2, 29.1% 3,5-(H2N)2C6H3Cl, and traces of m-Cl2C6H4.

IT **108-70-3**
(amination of, chloroanilines from)

RN 108-70-3 HCAPLUS

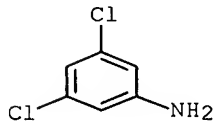
CN Benzene, 1,3,5-trichloro- (8CI, 9CI) (CA INDEX NAME)



IT **626-43-7P**
(preparation of)

RN 626-43-7 HCAPLUS

CN Benzenamine, 3,5-dichloro- (9CI) (CA INDEX NAME)



IC C07C087-60

CC 25-4 (Noncondensed Aromatic Compounds)

IT **108-70-3**
(amination of, chloroanilines from)

IT **626-43-7P** 33786-89-9P
(preparation of)

L64 ANSWER 48 OF 55 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1979:38660 HCAPLUS Full-text

DOCUMENT NUMBER: 90:38660

TITLE: 3,5-Dihaloanilines

INVENTOR(S): Jersak, Ulrich; Scheuermann, Horst

PATENT ASSIGNEE(S): BASF A.-G., Fed. Rep. Ger.

SOURCE: Ger. Offen., 9 pp.
CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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DE 2720316	A1	19781116	DE 1977-2720316	1977 0506 <--
DE 2720316	C2	19820401		
JP 53137921	A2	19781201	JP 1978-44880	1978 0418 <--
BE 866662	A1	19781103	BE 1978-187352	1978 0503 <--
FR 2389596	A1	19781201	FR 1978-13075	1978 0503 <--
FR 2389596	B1	19830718		
CH 633252	A	19821130	CH 1978-4854	1978 0503 <--
GB 1601746	A	19811104	GB 1978-17960	1978 0505 <--

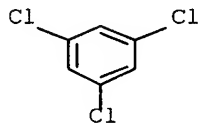
PRIORITY APPLN. INFO.: DE 1977-2720316 A 1977 0506 <--

AB 3,5-RR1C6H3NH2 (R, R1 = halo) were prepared by treating 1,3,5-trihalobenzenes with NH3 in the presence of a Cu catalyst. Thus, 25 parts 1,3,5-Cl3C6H3 and 1 part Cu(OAc)2.H2O treated with 50 parts NH3 for 25 h at 120° gave 85% 3,5-Cl2C6H3NH2.

IT **108-70-3**
(amination of, catalyst for)

RN 108-70-3 HCAPLUS

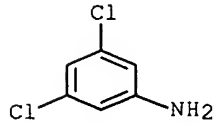
CN Benzene, 1,3,5-trichloro- (8CI, 9CI) (CA INDEX NAME)



IT **626-43-7P**
(preparation of, by amination of trichlorobenzene)

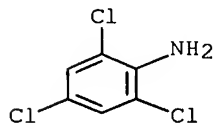
RN 626-43-7 HCAPLUS

CN Benzenamine, 3,5-dichloro- (9CI) (CA INDEX NAME)

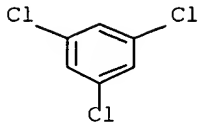


IC C07C087-60
CC 25-4 (Noncondensed Aromatic Compounds)
IT **108-70-3** 626-39-1
(amination of, catalyst for)
IT **626-43-7P**
(preparation of, by amination of trichlorobenzene)

L64 ANSWER 49 OF 55 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1978:546530 HCAPLUS Full-text
DOCUMENT NUMBER: 89:146530
TITLE: Synthesis of carbon-14-labeled environmental chemicals
AUTHOR(S): Sandrock, K.; Attar, A.; Bieniek, D.; Klein, W.; Korte, F.
CORPORATE SOURCE: Inst. Oekol. Chem., Ges. Strahlen- und Umweltforsch. m.b.H., Munich, Fed. Rep. Ger.
SOURCE: Journal of Labelled Compounds and Radiopharmaceuticals (**1978**), 14(2), 197-204
CODEN: JLCRD4; ISSN: 0362-4803
DOCUMENT TYPE: Journal
LANGUAGE: German
AB Chlorination (N-chlorosuccinimide) (NCS) of PhNH2-14C gave 80% 2,4,6-Cl3C6H2NH2-14C whereas chlorination of PhNHAc-14C gave, according to the amount of NCS used, 96% 2,4-Cl2C6H3NHAc-14C or 66% 4-ClC6H4NHAc-14C and 26% 2-ClC6H4NHAc-14C. Gomberg-Bachmann or Cadogan reaction of diazotized 14C labeled chloroanilines with different chlorobenzenes gave 14C labeled di-, tri-, and pentachlorobiphenyls. E.g., diazotized 2,4-Cl2C6H3NHAc-14C with 1,3,5-Cl3C6H3 gave 29% 2,2',4,4',6-pentachlorobiphenyl-14C. On boiling anilinediazonium-14C sulfate, PhOH-14C was prepared, which was chlorinated (NCS) to give 63.2% 2,4,6-Cl3C6H2OH-14C. Cl6C6-14C and Cl5C6NO2-14C were prepared by chlorination (Cl/ClSO3H) of PhNO2-14C. Chloralkylene 9-14C was obtained by Friedel-Crafts alkylation of 2,4'-dichlorobiphenyl-14C with Me2CHCl.
IT **40189-47-7P**
(preparation of)
RN 40189-47-7 HCAPLUS
CN Benzenamine-14C, 2,4,6-trichloro- (9CI) (CA INDEX NAME)

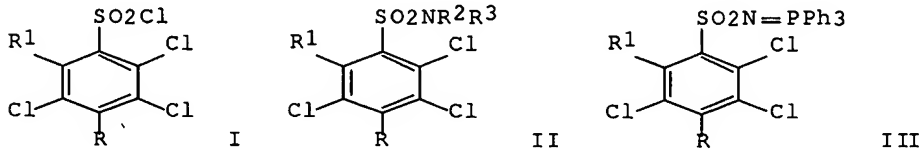


IT **108-70-3**
(reaction of, with diazotized chloroanilines, in preparation of carbon-14 labeled chlorobiphenyl)
RN 108-70-3 HCAPLUS
CN Benzene, 1,3,5-trichloro- (8CI, 9CI) (CA INDEX NAME)



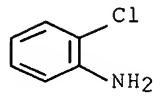
CC 25-10 (Noncondensed Aromatic Compounds)
IT **40189-47-7P** 67471-26-5P 67471-28-7P 67471-29-8P
67471-30-1P 67479-21-4P 67729-45-7P 67729-48-0P
(preparation of)
IT 106-46-7 **108-70-3** 108-90-7, reactions
(reaction of, with diazotized chloroanilines, in preparation of carbon-14 labeled chlorobiphenyl)

L64 ANSWER 50 OF 55 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1976:559576 HCAPLUS Full-text
DOCUMENT NUMBER: 85:159576
TITLE: Studies in the chemistry of polyhalobenzene compounds. The synthesis and reactivity of 2,3,5,6- and 2,3,4,5-tetrachlorobenzenesulfonyl chlorides and related compounds
AUTHOR(S): Chivers, Geoffrey E.; Cremlyn, Richard J. W.; Cronjie, Theo N.; Martin, Roger A.
CORPORATE SOURCE: Sch. Nat. Sci., Hatfield Polytech., Hatfield/Hertfordshire, UK
SOURCE: Australian Journal of Chemistry (**1976**), 29(7), 1573-82
CODEN: AJCHAS; ISSN: 0004-9425
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 85:159576
GI

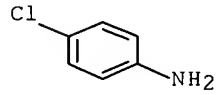


I II III

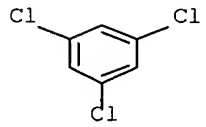
AB Polychlorobenzenesulfonyl chlorides I (R = Cl, H; R1 = H, Cl) were prepared from the sulfonic acids and PCl5 and amidated to yield sulfonamides II (R2 = H, Me; R3 = PhCH2, Me, Ph, substituted phenyl). I reacted with NaN3 and the sulfonyl azides obtained were treated with Ph3P to give iminophosphoranes III.
IT **95-51-2 106-47-8**
(amidation of polychlorobenzenesulfonyl chlorides by)
RN 95-51-2 HCAPLUS
CN Benzenamine, 2-chloro- (9CI) (CA INDEX NAME)



RN 106-47-8 HCAPLUS
CN Benzenamine, 4-chloro- (9CI) (CA INDEX NAME)

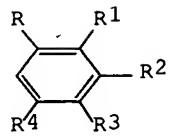


IT **108-70-3P**
(by desulfonation of trichlorobenzenesulfonic hydrazide)
RN 108-70-3 HCAPLUS
CN Benzene, 1,3,5-trichloro- (8CI, 9CI) (CA INDEX NAME)

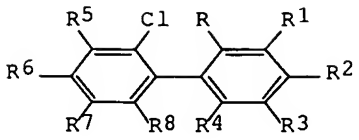


CC 25-13 (Noncondensed Aromatic Compounds)
IT 62-53-3, reactions 88-74-4 **95-51-2** 99-09-2
100-46-9 104-94-9 **106-47-8** 109-73-9 124-40-3,
reactions 504-29-0 7664-41-7, reactions
(amidation of polychlorobenzenesulfonyl chlorides by)
IT **108-70-3P**
(by desulfonation of trichlorobenzenesulfonic hydrazide)

L64 ANSWER 51 OF 55 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1976:477777 HCAPLUS Full-text
DOCUMENT NUMBER: 85:77777
TITLE: Synthesis and structural study of some isomers of polychlorinated biphenyls
AUTHOR(S): Erb, Francoise; Pommery, Jean; Van Aerde, Christine; Vermeersch, Gaston
CORPORATE SOURCE: Lab. Hydrol. Toxicol., Fac. Pharm., Lille, Fr.
SOURCE: Bulletin de la Societe Chimique de France (**1976**), (5-6, Pt. 2), 964-8
CODEN: BSCFAS; ISSN: 0037-8968
DOCUMENT TYPE: Journal
LANGUAGE: French
OTHER SOURCE(S): CASREACT 85:77777
GI



I



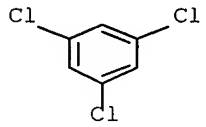
II

AB Chloroanilines were diazotized and condensed with benzenes I (R, R1, R2, R3, and R4 are independently H or Cl) to yield fourteen resp. chlorobiphenyls II (R5, R6, R7, and R8 are independently H or Cl).

IT **108-70-3**
(condensation reaction of, with chlorobenzediazonium salts, chlorobiphenyls from)

RN 108-70-3 HCAPLUS

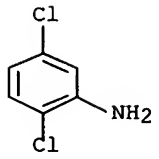
CN Benzene, 1,3,5-trichloro- (8CI, 9CI) (CA INDEX NAME)



IT **95-82-9 608-27-5 634-93-5**
636-30-6
(diazotization and condensation reaction of, with benzene and chlorobenzenes, chlorobiphenyls from)

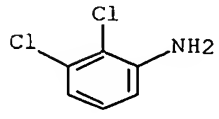
RN 95-82-9 HCAPLUS

CN Benzenamine, 2,5-dichloro- (9CI) (CA INDEX NAME)



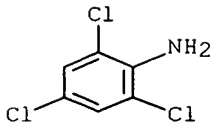
RN 608-27-5 HCAPLUS

CN Benzenamine, 2,3-dichloro- (9CI) (CA INDEX NAME)

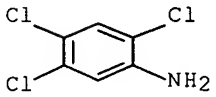


RN 634-93-5 HCAPLUS

CN Benzenamine, 2,4,6-trichloro- (9CI) (CA INDEX NAME)

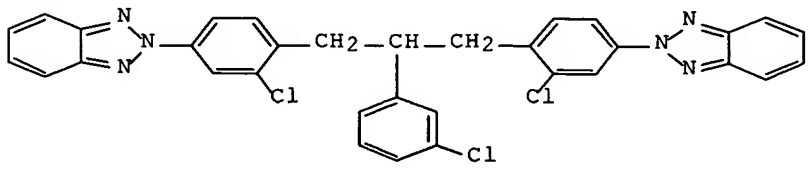


RN 636-30-6 HCAPLUS
CN Benzenamine, 2,4,5-trichloro- (9CI) (CA INDEX NAME)



CC 25-3 (Noncondensed Aromatic Compounds)
IT 71-43-2, reactions 95-50-1 106-46-7 **108-70-3**
634-66-2
(condensation reaction of, with chlorobenzediazonium salts, chlorobiphenyls from)
IT **95-82-9 608-27-5 634-93-5**
636-30-6
(diazotization and condensation reaction of, with benzene and chlorobenzenes, chlorobiphenyls from)

L64 ANSWER 52 OF 55 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1976:405562 HCAPLUS Full-text
DOCUMENT NUMBER: 85:5562
TITLE: Anil synthesis. Part 12. On the preparation of 1,2,3-triarylpropane compounds
AUTHOR(S): Coviello, Vincenzo; Siegrist, Adolf E.
CORPORATE SOURCE: Org.-Chem. Inst., Univ. Freiburg, Fribourg, Switz.
SOURCE: Helvetica Chimica Acta (**1976**), 59(3), 802-19
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 85:5562
GI



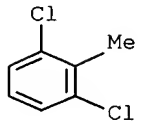
I

AB Schiff bases of aromatic aldehydes react with 2 mole-equivs. 2,5-Cl2C6H3Me or 2 mole-equivs. 2-(3-chloro-4-methylphenyl)-2H- benzotriazoles, -2H-naphtho[1,2-d]triazoles, -oxazoles, or -benzoxazoles in presence of DMF and KOH to give 1,2,3-triarylpropanes, e.g., I.

IT **118-69-4**
(reaction with Schiff bases)

RN 118-69-4 HCAPLUS

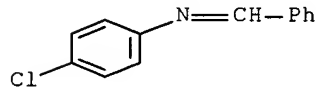
CN Benzene, 1,3-dichloro-2-methyl- (9CI) (CA INDEX NAME)



IT **780-21-2 10480-32-7 15485-22-0**
17099-07-9 17099-20-6 38608-21-8
(reaction with o-chlorotoluene derivs.)

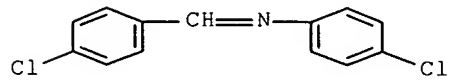
RN 780-21-2 HCAPLUS

CN Benzenamine, 4-chloro-N-(phenylmethylene)- (9CI) (CA INDEX NAME)



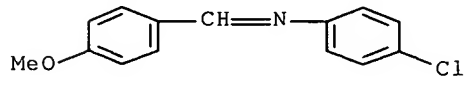
RN 10480-32-7 HCAPLUS

CN Benzenamine, 4-chloro-N-[(4-chlorophenyl)methylene]- (9CI) (CA INDEX NAME)



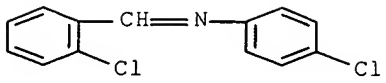
RN 15485-22-0 HCAPLUS

CN Benzenamine, 4-chloro-N-[(4-methoxyphenyl)methylene]- (9CI) (CA INDEX NAME)

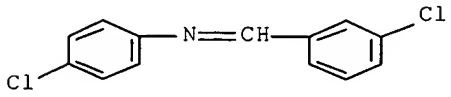


RN 17099-07-9 HCAPLUS

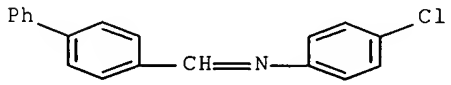
CN Benzenamine, 4-chloro-N-[(2-chlorophenyl)methylene]- (9CI) (CA INDEX NAME)



RN 17099-20-6 HCAPLUS
CN Benzenamine, 4-chloro-N-[(3-chlorophenyl)methylene]- (9CI) (CA INDEX NAME)



RN 38608-21-8 HCAPLUS
CN Benzenamine, N-([1,1'-biphenyl]-4-ylmethylene)-4-chloro- (9CI) (CA INDEX NAME)



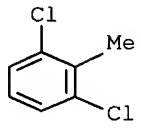
CC 28-11 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 25
IT 95-73-8 **118-69-4** 1124-05-6 19398-61-9 36843-34-2
38610-35-4 42196-67-8 59425-93-3
(reaction with Schiff bases)
IT **780-21-2** 6206-78-6 **10480-32-7**
15485-22-0 17099-07-9 17099-20-6
38608-21-8 38662-76-9 41855-64-5
(reaction with o-chlorotoluene derivs.)

L64 ANSWER 53 OF 55 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1975:86163 HCAPLUS Full-text
DOCUMENT NUMBER: 82:86163
TITLE: Synthesis of 2,6-dichlorobenzaldoxime from 4-nitrotoluene
AUTHOR(S): Buchwald, P.; Domnariu, F.
CORPORATE SOURCE: Chem. Pharm. Res. Inst., Cluj, Rom.
SOURCE: Revue Roumaine de Chimie (**1974**), 19(7), 1221-5
CODEN: RRCHAX; ISSN: 0035-3930
DOCUMENT TYPE: Journal
LANGUAGE: English
AB 2,6-Cl2C6H3CH:NOH (I) was prepared from 4-MeC6H4-NO2, which was chlorinated with Cl in the presence of SbCl5 to give a mixture of 3,4-ClMeC6H4R (II; R = NO2), 3,5,4-Cl2Me-C6H2R (III; R = NO2) and 2,3,5,4-Cl3MeC6HR (IV; R = NO2), which was reduced to a mixture of II (R = NH2), III (R = NH2), and IV (R =

NH2), which was converted by diazotization into a mixture of II (R = H), III (R = H), and IV (R = H). 2,6-Cl2-C6H3Me was separated from the mixture by fractionation and chlorinated in the presence of NCCMe2N:NCMe2CN to give a mixture of 2,6-Cl2C6H3CH2Cl, 2,6-Cl2C6H3CHCl2, and 2,6-Cl2C6-H3CCl3, which was hydrolyzed with H2SO4 and reacted with HONH2.HCl to give 2,4-Cl2C6H3CH2OH, I, and 2,6-Cl2C6H3-CO2H, resp. I was separated by treating the mixture with NaHCO3, then with NaOH.

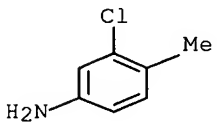
IT **118-69-4P**
(preparation and chlorination of)

RN 118-69-4 HCAPLUS
CN Benzene, 1,3-dichloro-2-methyl- (9CI) (CA INDEX NAME)

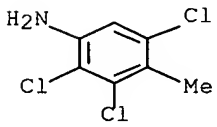


IT **95-74-9P 39053-35-5P 54730-35-7P**
(preparation and deamination of isomeric mixture containing)

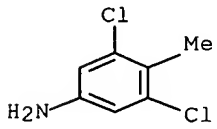
RN 95-74-9 HCAPLUS
CN Benzenamine, 3-chloro-4-methyl- (9CI) (CA INDEX NAME)



RN 39053-35-5 HCAPLUS
CN Benzenamine, 2,3,5-trichloro-4-methyl- (9CI) (CA INDEX NAME)

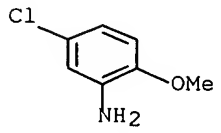


RN 54730-35-7 HCAPLUS
CN Benzenamine, 3,5-dichloro-4-methyl- (9CI) (CA INDEX NAME)

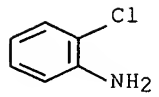


CC 25-15 (Noncondensed Aromatic Compounds)
IT **118-69-4P**
(preparation and chlorination of)
IT **95-74-9P 39053-35-5P 54730-35-7P**
(preparation and deamination of isomeric mixture containing)

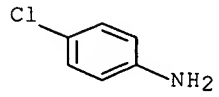
L64 ANSWER 54 OF 55 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1973:437517 HCAPLUS Full-text
DOCUMENT NUMBER: 79:37517
TITLE: Preparation of organic compounds labeled by chlorine-38. I. Inorganic yields of 38Cl in Szilard-Chalmer reactions of aromatic chloro derivatives
AUTHOR(S): Kim, You Sun
CORPORATE SOURCE: Chem. Div., At. Energy Res. Inst., Seoul, S. Korea
SOURCE: Journal of the Korean Nuclear Society (**1973**), 5(1), 44-54
CODEN: WJHKAW; ISSN: 0372-7327
DOCUMENT TYPE: Journal
LANGUAGE: English
AB To clarify an effective procedure of labeling organic chloro compds. by 38Cl, chlorobenzene derivs. (7 kinds), chloronitrobenzenes (6 kinds), chloroanisoles (2 kinds), chloroanilines (3 kinds), chlorotoluenes (3 kinds), benzyl chlorides (4 kinds), and other comparing samples (3 kinds) were irradiated in the TRIGA Mark-II research and the inorg. 38Cl yields were compared with the irradiation times after extracting the inorg. portion with an aqueous alkali solution The relative change between the inorg. 38Cl yield and the irradiation time depended a great deal on the state of the sample; a solid sample gave a lower and steady inorg. yield. The inorg. 38Cl yield decreased in the order chlorobenzene derivs. < chlorotoluene < benzyl chloride < chlorocyclohexane < chloronitrobenzene < chloroaniline. Among the compds. of similar chemical structure, ortho and para isomers gave similar inorg. yields. A linear relation was observed between the inorg. 38Cl yield of homo functional compds. and the number of Cl atoms on the benzene ring. Generally, polychloro substituted derivs. gave a higher yield than those less substituted derivs. The results are discussed and the feasibility of these results for labeling purposes was criticized.
IT **95-03-4 95-51-2 106-47-8**
108-70-3 554-00-7 33353-68-3
42138-72-7
(neutron irradiation of, yield of inorg. chlorine-38 in, labeling by Szilard-Chalmers process in relation to)
RN 95-03-4 HCAPLUS
CN Benzenamine, 5-chloro-2-methoxy- (9CI) (CA INDEX NAME)



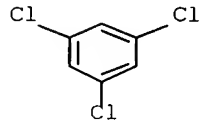
RN 95-51-2 HCAPLUS
CN Benzenamine, 2-chloro- (9CI) (CA INDEX NAME)



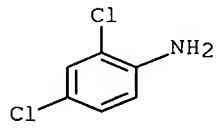
RN 106-47-8 HCAPLUS
CN Benzenamine, 4-chloro- (9CI) (CA INDEX NAME)



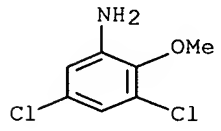
RN 108-70-3 HCAPLUS
CN Benzene, 1,3,5-trichloro- (8CI, 9CI) (CA INDEX NAME)



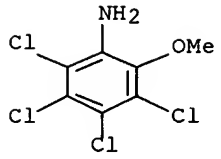
RN 554-00-7 HCAPLUS
CN Benzenamine, 2,4-dichloro- (9CI) (CA INDEX NAME)



RN 33353-68-3 HCAPLUS
CN Benzenamine, 3,5-dichloro-2-methoxy- (9CI) (CA INDEX NAME)

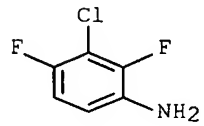


RN 42138-72-7 HCAPLUS
CN Benzenamine, 2,3,4,5-tetrachloro-6-methoxy- (9CI) (CA INDEX NAME)

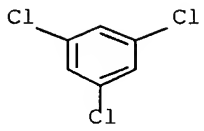


CC 75-10 (Nuclear Phenomena)
Section cross-reference(s): 22, 25
IT 57-15-8 76-83-5 87-61-6 88-73-3 89-21-4 **95-03-4**
95-49-8 **95-51-2** 95-94-3 100-00-5 100-14-1
100-44-7 104-82-5 106-43-4 106-46-7 **106-47-8**
108-41-8 **108-70-3** 108-90-7, reactions 120-82-1
121-73-3 541-73-1 542-18-7 **554-00-7** 611-06-3
620-19-9 **33353-68-3 42138-72-7**
(neutron irradiation of, yield of inorg. chlorine-38 in, labeling by Szilard-Chalmers process in relation to)

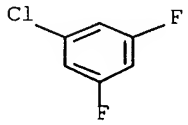
L64 ANSWER 55 OF 55 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1972:500961 HCAPLUS Full-text
DOCUMENT NUMBER: 77:100961
TITLE: Fluorination of 1,2,3-, 1,2,4-, and 1,3,5-trihalobenzenes with potassium fluoride in dimethyl sulfone
AUTHOR(S): Shiley, R. H.; Dickerson, D. R.; Finger, G. C.
CORPORATE SOURCE: Illinois State Geol. Surv., Urbana, IL, USA
SOURCE: Journal of Fluorine Chemistry (**1972**), Volume Date 1972-1973, 2(1), 19-26
CODEN: JFLCAR; ISSN: 0022-1139
DOCUMENT TYPE: Journal
LANGUAGE: English
AB 1,2,3- (I), 1,2,4- (II), and 1,3,5-Trifluorobenzene (III) were prepared (12.8, 8.3, and 56.2%, resp.) by reaction of the corresponding trichlorobenzenes with KF or KF-CsF mixts. in Me2SO2. Improved yields of I (23.9%) and II (34.0%) were obtained from chlorofluorobenzene intermediates which were obtained by controling the reaction variables. In the halogen exchange reaction medium, polyfluorobenzenes were unstable.
IT **2613-34-5**
(diazotization of)
RN 2613-34-5 HCAPLUS
CN Benzenamine, 3-chloro-2,4-difluoro- (9CI) (CA INDEX NAME)



IT **108-70-3**
(fluorination of, with potassium fluoride)
RN 108-70-3 HCAPLUS
CN Benzene, 1,3,5-trichloro- (8CI, 9CI) (CA INDEX NAME)



IT **1435-43-4P**
(preparation of)
RN 1435-43-4 HCAPLUS
CN Benzene, 1-chloro-3,5-difluoro- (7CI, 8CI, 9CI) (CA INDEX NAME)



CC 25-3 (Noncondensed Aromatic Compounds)
IT **2613-34-5**
(diazotization of)
IT 87-61-6 **108-70-3** 120-82-1 2367-91-1
(fluorination of, with potassium fluoride)
IT 348-51-6P 348-59-4P 352-33-0P 367-11-3P 367-23-7P
372-18-9P 372-38-3P 462-06-6P 625-98-9P 696-02-6P
1435-43-4P 1435-44-5P 1435-46-7P 1435-48-9P
1435-49-0P 1489-53-8P 2268-05-5P 36556-47-5P 36556-50-0P
38361-37-4P
(preparation of)